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FILE LAST UPDATED: 6 Jan 2008  (20080106/ED)

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http://www.cas.org/infopolicy.html

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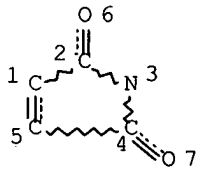


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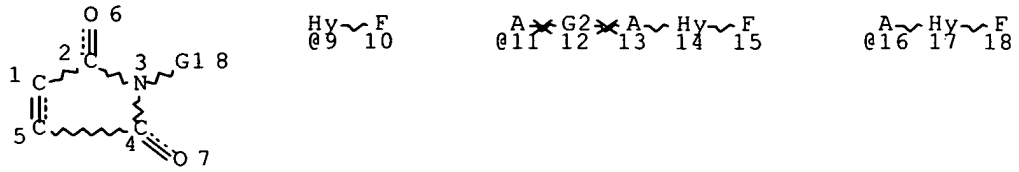

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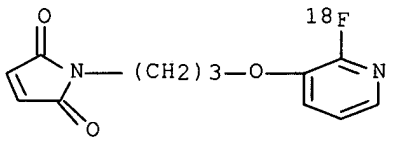
L17 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:159447 CAPLUS Full-text
DOCUMENT NUMBER: 142:388335
TITLE: 1-[3-(2-[18F]Fluoropyridin-3-yloxy)propyl]pyrrole-2,5-dione: Design, Synthesis, and Radiosynthesis of a New [18F]Fluoropyridine-Based Maleimide Reagent for the Labeling of Peptides and Proteins
AUTHOR(S): De Bruin, Beatrice; Kuhnast, Bertrand; Hinnen, Francoise; Yaouancq, Loiec; Amessou, Mohamed; Johannes, Ludger; Samson, Alain; Boisgard, Raphaeel; Tavitian, Bertrand; Dolle, Frederic
CORPORATE SOURCE: Service Hospitalier Frederic Joliot, Departement de Recherche Medicale, CEA/DSV, Orsay, F-91401, Fr.
SOURCE: Bioconjugate Chemistry (2005), 16(2), 406-420
CODEN: BCCHES; ISSN: 1043-1802
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB FPyME (1-[3-(2-fluoropyridin-3-yloxy)propyl]pyrrole-2,5-dione) was designed as a [18F]fluoropyridine-based maleimide reagent for the prosthetic labeling of peptides and proteins via selective conjugation with a thiol (sulfhydryl) function. Its pyridinyl moiety carries the radioactive halogen (fluorine-18) which can be efficiently incorporated via a nucleophilic heteroarom.

substitution, and its maleimido function ensures the efficient alkylation of a free thiol function as borne by cysteine residues. [18F]FPyME (HPLC-purified) was prepared in 17-20% non-decay-corrected yield, based on starting [18F]fluoride, in 110 min using a three-step radiochem. pathway. The developed procedure involves (1) a high-yield nucleophilic heteroarom. ortho-radiofluorination on [3-(3-tert-butoxycarbonylaminopropoxy)pyridin-2-yl]trimethylammonium trifluoromethanesulfonate as the fluorine-18 incorporation step, followed by (2) rapid and quant. TFA-induced removal of the N-Boc-protective group and (3) optimized maleimide formation using N-methoxycarbonylmaleimide. Typically, 4.8-6.7 GBq (130-180 mCi) of radiochem. pure [18F]FPyME ([18F]-1) could be obtained after semipreparative HPLC in 110 min starting from a cyclotron production batch of 33.3 GBq (900 mCi) of [18F]fluoride (overall radiochem. yields, based on starting [18F]fluoride: 28-37% decay-corrected). [18F]FPyME ([18F]-1) was first conjugated with a small model hexapeptide ((N-Ac)KAAAAC), confirming the excellent chemoselectivity of the coupling reaction (CH2SH vs. CH2NH2) and then conjugated with two 8-kDa proteins of interest, currently being developed as tumor imaging agents (c-AFIM-0 and c-STxB). Conjugation was achieved in high yields (60-70%, isolated and non-decay-corrected) and used optimized, short-time reaction conditions (a 1/9 (volume/volume) mixture of DMSO and 0.05 M aq Tris NaCl buffer (pH 7.4) or 0.1 M aq PBS (pH 8), at room temperature for 10 min) and purification conditions (a gel filtration using a Sephadex NAP-10 cartridge or a SuperDex Peptide HR 10/30 column), both compatible with the chemical stability of the proteins and the relatively short half-life of the radioisotope concerned. The whole radiosynthetic procedure, including the preparation of the fluorine-18-labeled reagent, the conjugation with the protein and the final purification took 130-140 min. [18F]FPyME ([18F]-1) represents a new, valuable, thiol-selective, fluorine-18-labeled reagent for the prosthetic labeling with fluorine-18 of peptides and proteins. Because of its excellent chemoselectivity, [18F]FPyME offers an interesting alternative to the use of the nonselective carboxylate and amine-reactive [18F]reagents and can therefore advantageously be used for the design and development of new peptide- and protein-based radiopharmaceuticals for PET.

IT 640749-66-2DP, complexes with proteins 640749-66-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(1-[3-(2-[18F]fluoropyridin-3-yloxy)propyl]pyrrole-2,5-dione: preparation of
new [18F]fluoropyridine-based maleimide reagent for labeling of peptides and proteins)

RN 640749-66-2 CAPLUS
CN 1H-Pyrrole-2,5-dione, 1-[3-[[2-(fluoro-18F)-3-pyridinyl]oxy]propyl]- (9CI) (CA INDEX NAME)



RN 640749-66-2 CAPLUS
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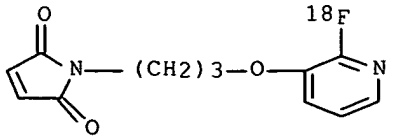

REFERENCE COUNT: 81 THERE ARE 81 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:20709 CAPLUS Full-text
DOCUMENT NUMBER: 140:89682
TITLE: Fluorine-18-marked peptides having affinity for negatively charged cell surfaces for use in diagnosis
INVENTOR(S): Sanson, Alain; Ochsenbein, Francoise; Dolle, Frederic
PATENT ASSIGNEE(S): Commissariat a l'Energie Atomique, Fr.; Universite Pierre et Marie Curie (Paris VI)
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004003016	A2	20040108	WO 2003-FR2027	20030630
WO 2004003016	A3	20040408		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
FR 2841558	A1	20040102	FR 2002-8204	20020701
FR 2841558	B1	20040813		
CA 2491344	A1	20040108	CA 2003-2491344	20030630
AU 2003259311	A1	20040119	AU 2003-259311	20030630
EP 1517919	A2	20050330	EP 2003-761669	20030630
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006510577	T	20060330	JP 2004-516900	20030630
US 2006233706	A1	20061019	US 2004-518382	20041229

PRIORITY APPLN. INFO.: FR 2002-8204 A 20020701
WO 2003-FR2027 W 20030630

OTHER SOURCE(S): MARPAT 140:89682

AB The invention concerns peptides containing F18, F18-containing reagents for labeling peptides with F18, and the use of the F18-labeled peptides for diagnosis, e.g., for use in PET. The peptide derivs. bind to neg. charges on cell surfaces, such as phosphatidylserine on the surfaces of apoptotic cells, or on microvesicles in the blood. Peptides of the invention were labeled with fluorescein and injected into the tail vein of a rat infarct model. The apoptotic heart cells were clearly labeled more intensely in the infarct model

that in the normal control. These same peptides, which were labeled with F18, could be used similarly for PET anal. of human infarcts.

IT 640749-66-2P 640749-70-8P 640749-71-9P
640749-72-0P 640749-73-1P 640749-74-2P
640749-75-3P 640749-76-4P 640749-77-5P
640749-78-6P 640749-79-7P 640749-80-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(fluorine-18-marked peptides having affinity for neg. charged cell surfaces for use in diagnosis)

RN 640749-66-2 CAPLUS
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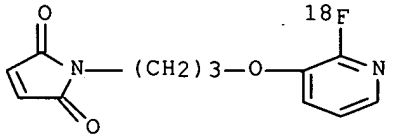

RN 640749-70-8 CAPLUS
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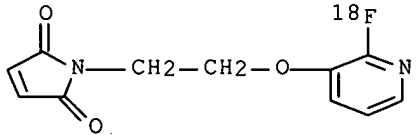

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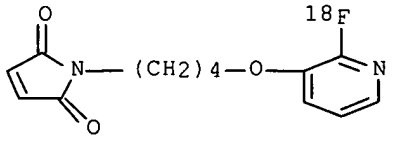

RN 640749-72-0 CAPLUS
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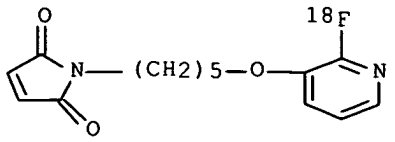

RN 640749-73-1 CAPLUS
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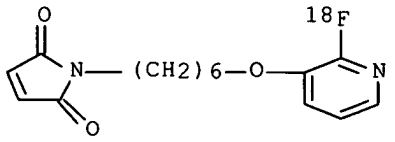

RN 640749-74-2 CAPLUS
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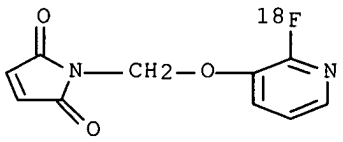

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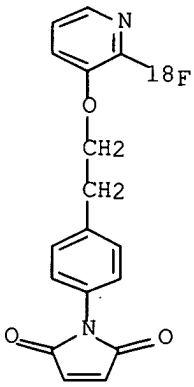

RN 640749-76-4 CAPLUS
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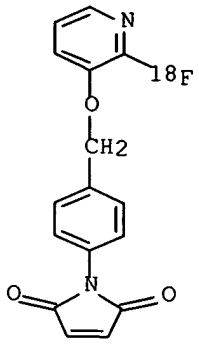

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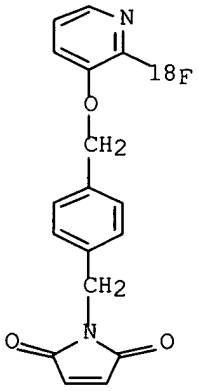

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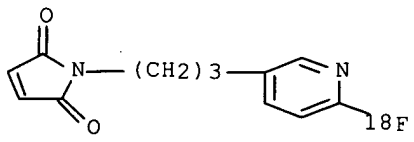

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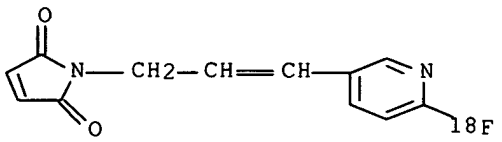

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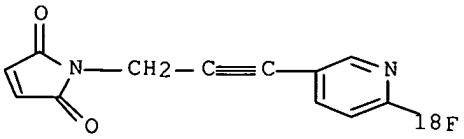


L17 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:20684 CAPLUS Full-text
DOCUMENT NUMBER: 140:77021
TITLE: Preparation of [18F]-labeled maleimides, their use for marking macromolecules for medical imaging
INVENTOR(S): Dolle, Frederic
PATENT ASSIGNEE(S): Commissariat a l'Energie Atomique, Fr.
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004002984	A2	20040108	WO 2003-FR2028	20030630
WO 2004002984	A3	20040422		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
FR 2841554	A1	20040102	FR 2002-8203	20020701
CA 2491193	A1	20040108	CA 2003-2491193	20030630
AU 2003259312	A1	20040119	AU 2003-259312	20030630

EP 1517903	A2	20050330	EP 2003-761670	20030630
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006504640	T	20060209	JP 2004-516901	20030630
US 2005249662	A1	20051110	US 2004-517612	20041222
PRIORITY APPLN. INFO.:			FR 2002-8203	A 20020701
			WO 2003-FR2028	W 20030630

OTHER SOURCE(S): MARPAT 140:77021
GI

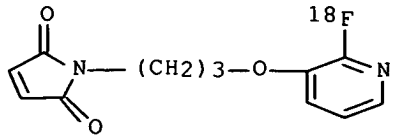
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB [18F]-Maleimides I [wherein: X = (X1)m; Y = (Y1)n; m = 0 to 10; n = 1 to 10; Y1 = (un)substituted monocyclic or bicyclic heterocyclyl; X1 = (U)a-((CR1R2)b-(V)c)d-((CR3R4)e-(W)f)g; a, b, c, d, e, f, g = independently 0 to 10; U, V and W = independently NH and derivs., O, S, ethynyl, C:O, C:S, C=NH and derivs., C(=O)O, (C=S)S, C(=NH)NH and derivs. ,CH2 and derivs. ,CHOH and derivs., CHNH2 and derivs., etc.] were prepared for marking macromols. and complexes of I with macromols., and their use for anal., detection, or diagnosis by positron emission tomog. (PET). The advantages include fast and simple synthesis, and high yields of the [18F]-labeled product. For example, II was prepared by radiosynthesis by substitution reaction of tert-Bu [3-(2-nitropyridin-3-yloxy)propyl]carbamate with K[18F]F-Kryptofix K222 complex, BOC deprotection to [18F]aminofluoropyridine intermediate III, and substitution of N-methoxycarbonylmaleimide with III. [18F]-labeled peptide IV was prepared by reacting N-acetyl-L-Lys-L-Ala-L-Ala-L-Ala-L-Ala-L- Cys-amide with II. I and their complexes with macromols. are useful in medical imaging for detecting apoptosis, necrosis, and tumors by PET (no data).

IT 640749-66-2P, 1-[3-(2-[18F]Fluoropyridin-3-yloxy)propyl]pyrrole-2,5-dione 640749-70-8P, 1-[2-(2-[18F]Fluoropyridin-3-yloxy)ethyl]pyrrole-2,5-dione 640749-71-9P, 1-[4-(2-[18F]Fluoropyridin-3-yloxy)butyl]pyrrole-2,5-dione 640749-72-0P, 1-[5-(2-[18F]Fluoropyridin-3-yloxy)pentyl]pyrrole-2,5-dione 640749-73-1P, 1-[6-(2-[18F]Fluoropyridin-3-yloxy)hexyl]pyrrole-2,5-dione 640749-74-2P, 1-[(2-[18F]Fluoropyridin-3-yloxy)methyl]pyrrole-2,5-dione 640749-75-3P, 1-[4-[2-(2-[18F]Fluoropyridin-3-yloxy)ethyl]phenyl]pyrrole-2,5-dione 640749-76-4P, 1-[4-[(2-[18F]Fluoropyridin-3-yloxy)methyl]phenyl]pyrrole-2,5-dione 640749-77-5P, 1-[4-[(2-[18F]Fluoropyridin-3-yloxy)methyl]benzyl]pyrrole-2,5-dione 640749-78-6P, 1-[3-(6-[18F]Fluoropyridin-3-yl)propyl]pyrrole-2,5-dione 640749-79-7P, 1-[3-[6-[18F]Fluoropyridin-3-yl]allyl]pyrrole-2,5-dione 640749-80-0P, 1-[3-(6-[18F]Fluoropyridin-3-yl)prop-2-ynyl]pyrrole-2,5-dione
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(labeling agent; preparation of [18F]-labeled maleimides and their use for marking macromols. for medical imaging)

RN 640749-66-2 CAPLUS

CN 1H-Pyrrole-2,5-dione, 1-[3-[[2-(fluoro-18F)-3-pyridinyl]oxy]propyl]- (9CI) (CA INDEX NAME)



RN 640749-70-8 CAPLUS
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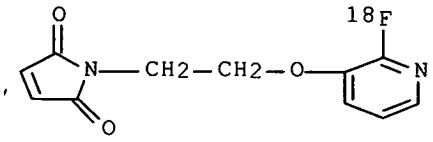
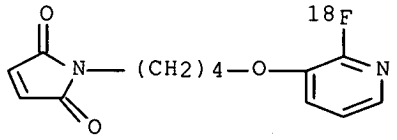


RN 640749-71-9 CAPLUS
CN 1H-Pyrrole-2,5-dione, 1-[4-[[2-(fluoro-18F)-3-pyridinyl]oxy]butyl]- (9CI) (CA INDEX NAME)



RN 640749-72-0 CAPLUS
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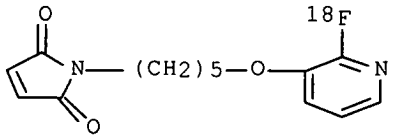
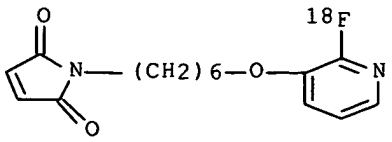
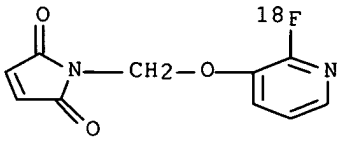


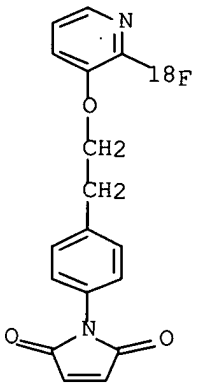
RN 640749-73-1 CAPLUS
CN 1H-Pyrrole-2,5-dione, 1-[6-[[2-(fluoro-18F)-3-pyridinyl]oxy]hexyl]- (9CI) (CA INDEX NAME)



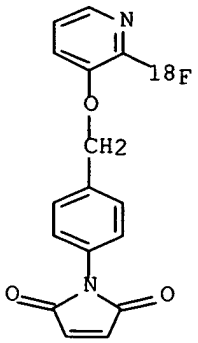
RN 640749-74-2 CAPLUS
CN 1H-Pyrrole-2,5-dione, 1-[[[2-(fluoro-18F)-3-pyridinyl]oxy]methyl]- (9CI) (CA INDEX NAME)



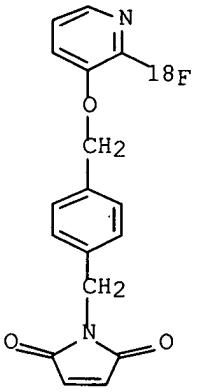
RN 640749-75-3 CAPLUS
CN 1H-Pyrrole-2,5-dione, 1-[4-[2-[[2-(fluoro-18F)-3-pyridinyl]oxy]ethyl]phenyl]- (9CI) (CA INDEX NAME)



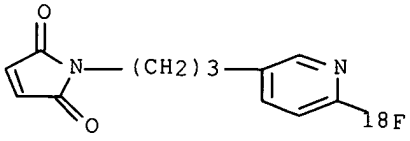
RN 640749-76-4 CAPLUS
CN 1H-Pyrrole-2,5-dione, 1-[4-[[[2-(fluoro-18F)-3-pyridinyl]oxy]methyl]phenyl]- (9CI) (CA INDEX NAME)



RN 640749-77-5 CAPLUS
CN 1H-Pyrrole-2,5-dione, 1-[[4-[[[2-(fluoro-18F)-3-pyridinyl]oxy]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



RN 640749-78-6 CAPLUS
CN 1H-Pyrrole-2,5-dione, 1-[3-[6-(fluoro-18F)-3-pyridinyl]propyl]- (9CI) (CA INDEX NAME)



RN 640749-79-7 CAPLUS
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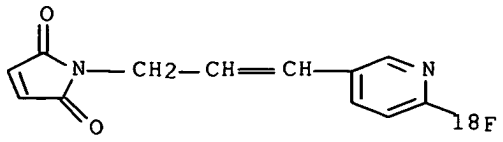
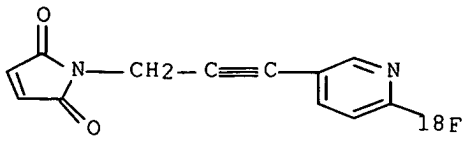


RN 640749-80-0 CAPLUS
CN 1H-Pyrrole-2,5-dione, 1-[3-[6-(fluoro-18F)-3-pyridinyl]-2-propynyl]- (9CI)
(CA INDEX NAME)



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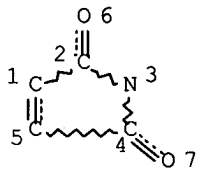
L3 STR



NODE ATTRIBUTES:
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DEFAULT ECLEVEL IS LIMITED

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NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE
L4 STR

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DEFAULT MLEVEL IS ATOM
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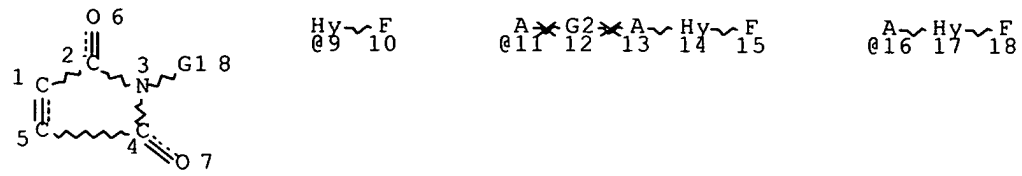
L10 STR



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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 3
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
L12 164 SEA FILE=REGISTRY SUB=L7 SSS FUL L10
L13 79 SEA FILE=CAPLUS ABB=ON PLU=ON L12
L14 30 SEA FILE=CAPLUS ABB=ON PLU=ON L13 AND (?LABEL? OR ?MARK? OR ?INDICAT? OR ?ISOTOP? OR 18F OR F18 OR F 18 OR 18 F)
L15 SCR 2039
L16 12 SEA FILE=REGISTRY SUB=L7 SSS FUL L15 AND L10
L17 3 SEA FILE=CAPLUS ABB=ON PLU=ON L16
L19 27 SEA FILE=CAPLUS ABB=ON PLU=ON L14 NOT L17

=> d l19 ibib abs hitind hitstr tot

L19 ANSWER 1 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:806265 CAPLUS Full-text
DOCUMENT NUMBER: 147:300697
TITLE: A Thiol-Reactive Fluorescence Probe Based on Donor-Excited Photoinduced Electron Transfer: Key Role of Ortho Substitution
AUTHOR(S): Matsumoto, Takuya; Urano, Yasuteru; Shoda, Takuji; Kojima, Hirotatsu; Nagano, Tetsuo
CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo, 113-0033, Japan
SOURCE: Organic Letters (2007), 9(17), 3375-3377
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:300697

AB We designed and synthesized a novel thiol-reactive fluorescence probe based on the BODIPY fluorophore. The fluorescence of this probe is strongly quenched by donor-excited photoinduced electron transfer (d-PeT) from BODIPY to maleimide, but after reaction with thiol, the fluorescence of BODIPY is restored, affording a 350-fold intensity increase.

CC 22-9 (Physical Organic Chemistry)
Section cross-reference(s): 9, 29, 73

IT Electron transfer
(intramol., photochem., fluorescence quenching mechanism before thiol labeling; a thiol-reactive fluorescence probe based on donor-excited photoinduced electron transfer and the key role of ortho substitution)

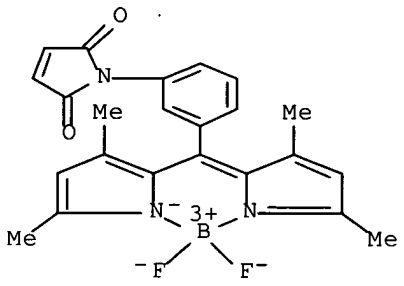
IT Fluorescent indicators
(of thiols; a thiol-reactive fluorescence probe based on donor-excited photoinduced electron transfer and the key role of ortho substitution)

IT 947328-69-0P 947328-71-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(a thiol-reactive fluorescence probe based on donor-excited photoinduced electron transfer and the key role of ortho substitution)

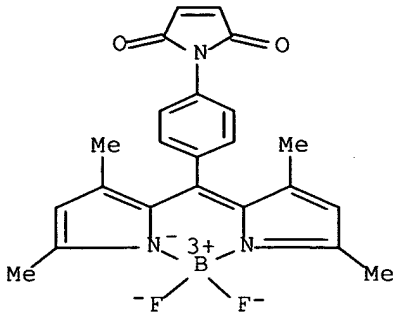
IT 929679-22-1P
RL: ARG (Analytical reagent use); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(target probe; a thiol-reactive fluorescence probe based on donor-excited photoinduced electron transfer and the key role of ortho substitution)

IT 947328-69-0P 947328-71-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(a thiol-reactive fluorescence probe based on donor-excited photoinduced electron transfer and the key role of ortho substitution)

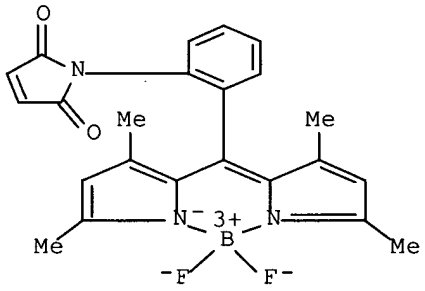
RN 947328-69-0 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



RN 947328-71-4 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



IT 929679-22-1P
RL: ARG (Analytical reagent use); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(target probe; a thiol-reactive fluorescence probe based on donor-excited photoinduced electron transfer and the key role of ortho substitution)
RN 929679-22-1 CAPLUS
CN Boron, [1-[2-[(3,5-dimethyl-1H-pyrrol-2-yl-κN)(3,5-dimethyl-2H-pyrrol-2-ylidene-κN)methyl]phenyl]-1H-pyrrole-2,5-dionato]difluoro-, (T-4)- (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:591913 CAPLUS Full-text
DOCUMENT NUMBER: 147:26523
TITLE: Methods for determining the redox status of proteins
INVENTOR(S): Lipscombe, Richard J.; Arthur, Peter Graeme
PATENT ASSIGNEE(S): The University of Western Australia, Australia; Proteomics International Pty. Ltd.
SOURCE: PCT Int. Appl., 43pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007059567	A1	20070531	WO 2006-AU1757	20061121

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: AU 2005-906469 A 20051122

AB A method for determining the redox status of a protein sample is described, the method comprising the steps of: (a) contacting the sample with a first label adapted to bind to at least one reduced cysteine group therein; (b) contacting the sample with a reducing agent to reduce at least one oxidized cysteine group therein; (c) contacting the sample with a second label adapted to bind to any reduced cysteine groups produced in step (b); and (d) determining the ratio of the signal from the first label to the signal from the second label wherein the ratio indicates the redox status. Reactive oxygen species-associated pathol. or disease can be assessed. Jurkat cells, +/- 2 mM H2O2 treatment for 5 min, were extracted with RBQ buffer (20% TCA in acetone, to trap thiol redox state). Protein samples were first labeled with Bodipy TMR cadaverine-iodoacetamide. Unreacted label was removed and samples were treated with the reducing agent 2-carboxyethylphosphine (TCEP) to reduce protein disulfides. The second label, Bodipy FL C1-iodoacetamide, was added with TCEP to react with newly exposed thiol groups. Proteins were separated on two dimensional electrophoresis gels and imaged with a fluoroimager. An automated spot detection program (ProGENESIS) was used to quantify the signal of reduced and oxidized proteins. For each labeled protein spot, a ratio of reduced to oxidized cysteine was calculated Four proteins were selected for further anal. because of differential staining.

CC 9-16 (Biochemical Methods)
Section cross-reference(s): 14

ST protein redox status detn label reducing agent cysteine; reactive oxygen species disease detn protein redox status; hydrogen peroxide treatment cell protein redox modification detn

IT Dyes
(Alexa Fluor, conjugates with cysteine-binding group; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Proteins
RL: ANT (Analyte); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study)
(HSU94832NID, detection of, as protein having redox modification due to Jurkat cell treatment with hydrogen peroxide; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Animal cell line
(JURKAT, treatment with hydrogen peroxide, detection of proteins having redox modification due to; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Dyes

(Oregon Green, conjugates with cysteine-binding group; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Liver, disease
(alc., as reactive oxygen species-associated disease, assessment of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Alcohols, biological studies
RL: BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(aliphatic, radicals, determination of protein modification by; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Ovalbumin
RL: BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(anal. of redox status of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Cell
(anal. of sample of extract of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Mitochondria
(anal. of sample of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Alzheimer's disease
Angina pectoris
Atherosclerosis
Cardiovascular system, disease
Coronary artery disease
Diabetes mellitus
Emphysema
Heart failure
Hypertension
Hypoxia
Myocardial infarction
Neoplasm
Parkinson's disease
Sleep apnea
(as reactive oxygen species-associated disease, assessment of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Redox potential
(biol.; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Bronchi, disease
Inflammation
(bronchitis, as reactive oxygen species-associated disease, assessment of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Embolism
(cerebral thromboembolism, as reactive oxygen species-associated disease, assessment of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Lung, disease
(chronic obstructive pulmonary disease, as reactive oxygen species-associated disease, assessment of; labels binding to

reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Fluorescent substances
Radioactive substances
(conjugates with cysteine-binding group, as label; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Thioredoxins
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(conjugates with protein, determination of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Enzymes, reactions
RL: ARG (Analytical reagent use); CAT (Catalyst use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(conjugates, with cysteine-binding group, as label; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Antibodies and Immunoglobulins
Proteins
RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(conjugates, with cysteine-binding group, as label; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Aging, animal
(degeneration related to, as reactive oxygen species-associated disease, assessment of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Heterogeneous nuclear ribonucleoproteins
RL: ANT (Analyte); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study)
(detection of, as protein having redox modification due to Jurkat cell treatment with hydrogen peroxide; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Reactive oxygen species
RL: BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(determination of protein modification by; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Animal tissue
(extract, anal. of sample of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Proteins
RL: ANT (Analyte); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study)
(far upstream element binding protein 1, detection of, as protein having redox modification; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT Embryo, animal, disease
(fetus, distress, as reactive oxygen species-associated disease, assessment of; labels binding to reduced cysteine groups of

proteins and reducing agent in determination of redox status of proteins)
IT Therapy
(for reactive oxygen species-associated disease, assessment of efficacy of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT Buffers
(in acid trapping proteins and quenching thiol-disulfide reactions; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT Human
Oxidation
Reducing agents
Reduction
Sample preparation
Samples
Sulfhydryl group
Test kits
(labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT Proteins
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); PRP (Properties); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT Sulfonic acids, biological studies
RL: BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT Mass spectrometry
(labels detectable by; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT Transplant and Transplantation
(liver, disease related to, as reactive oxygen species-associated disease, assessment of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT Proteins
RL: ANT (Analyte); BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); ANST (Analytical study); BIOL (Biological study); RACT (Reactant or reagent)
(modified, determination of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT Nervous system, disease
(neurotrauma, as reactive oxygen species-associated disease, assessment of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT Blood vessel, disease
(occlusion, peripheral, as reactive oxygen species-associated disease, assessment of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT Nanoparticles
(of gold, conjugates with cysteine-binding group, as label; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT Databases
(of redox values for proteins; labels binding to reduced

cysteine groups of proteins and reducing agent in determination of redox status
of proteins)
IT Acids, uses
RL: NUU (Other use, unclassified); USES (Uses)
(protein trapping with, in quenching thiol-disulfide reactions; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT Peroxides, biological studies
RL: BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(radicals, determination of protein modification by; labels binding to reduced cysteine groups of proteins and reducing agent in determination of
redox status of proteins)
IT Thiols, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactions with disulfides, quenching of, in pretreatment step; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT Disulfides
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactions with thiols, quenching of, in pretreatment step; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT Disease, animal
(reactive oxygen species-associated, assessment of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT Albumins, biological studies
RL: BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(serum, anal. of redox status of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status
of proteins)
IT Brain, disease
(stroke, as reactive oxygen species-associated disease, assessment of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT Liver
(transplant, disease related to, as reactive oxygen species-associated disease, assessment of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT 146368-16-3D, conjugates with cysteine-binding group
RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(Cy3, as label; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT 146368-14-1D, conjugates with cysteine-binding group
RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(Cy5, as label; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
IT 67-64-1, Acetone, uses
RL: NUU (Other use, unclassified); USES (Uses)
(TCA buffer in, in acid trapping proteins and quenching thiol-disulfide

reactions; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT 9001-03-0, Carbonic anhydrase 9001-05-2, Catalase 9001-63-2, Lysozyme 9001-75-6, Pepsin 9007-43-6, Cytochrome c, biological studies 9031-72-5, Alcohol dehydrogenase 9054-89-1, Superoxide dismutase
RL: BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(anal. of redox status of; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT 74-83-9, Methyl bromide, reactions 144-48-9, Iodoacetamide 152-34-1 541-59-3, Maleimide 587-85-9 1337-81-1, Vinylpyridine
RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(as cysteine-binding group of label; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT 773859-49-7, Bodipy FL N-(2-aminoethyl)maleimide 937803-30-0
RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(as first label; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT 81-88-9D, conjugates with cysteine-binding group 288-42-6D, Oxazole, pyridyl derivs., conjugates with cysteine-binding group 2321-07-5D, Fluorescein, conjugates with cysteine-binding group 7440-57-5D, Gold, nanoparticles, conjugates with cysteine-binding group 11120-54-0D, Oxadiazole, Ph derivs., conjugates with cysteine-binding group 17372-87-1D, Eosin, conjugates with cysteine-binding group 70281-37-7D, Tetramethylrhodamine, conjugates with cysteine-binding group 82354-19-6D, Texas Red, conjugates with cysteine-binding group 82446-52-4D, Lucifer yellow, conjugates with cysteine-binding group 138026-71-8D, Bodipy, conjugates with cysteine-binding group
RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(as label; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT 60-24-2, β-Mercaptoethanol 68-11-1, reactions 70-18-8, Reduced glutathione, reactions 998-40-3, Tributylphosphine 3483-12-3, Dithiothreitol 5961-85-3 7775-14-6, Sodium hydrosulfite 16940-66-2, Sodium borohydride
RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(as reducing agent; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT 217190-02-8 937803-31-1
RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(as second label; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT 76-03-9, Trichloroacetic acid, uses
RL: NUU (Other use, unclassified); USES (Uses)
(buffer, in acid trapping proteins and quenching thiol-disulfide reactions; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT 3170-83-0, Hydroperoxyl radical 3352-57-6, Hydroxyl radical, biological studies 7722-84-1, Hydrogen peroxide, biological studies 7782-44-7D, Oxygen, reactive species, biological studies 7790-92-3, Hypochlorous acid 10028-15-6, Ozone, biological studies 10102-43-9, Nitric oxide, biological studies 11062-77-4, Superoxide 19059-14-4, Peroxynitrite
RL: BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(determination of protein modification by; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT 52-90-4, L-Cysteine, biological studies
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); PRP (Properties); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(label binding to, in protein; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT 62607-44-7, Sulfenic acid
RL: BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT 56-89-3, Cystine, biological studies 70-18-8D, Glutathione, disulfide conjugates with protein
RL: BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT 498-40-8
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(reduction and labeling of, of protein; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT 7782-44-7, Oxygen, biological studies
RL: BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(singlet, determination of protein modification by; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

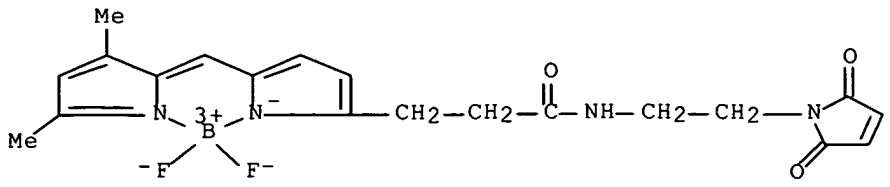
IT 9014-08-8
RL: ANT (Analyte); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study)
(α-, detection of, as protein having redox modification due to Jurkat cell treatment with hydrogen peroxide; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

IT 773859-49-7, Bodipy FL N-(2-aminoethyl)maleimide
RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(as first label; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)

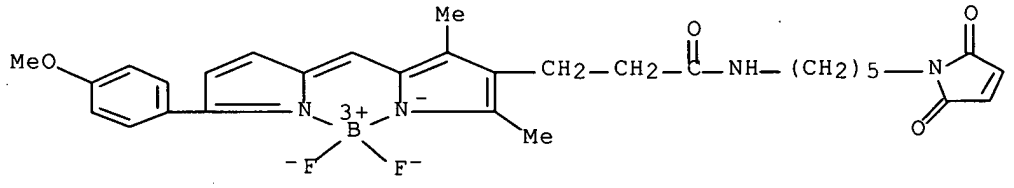
RN 773859-49-7 CAPLUS

CN Boron, [N-[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]-5-[(3,5-dimethyl-2H-pyrrol-2-ylidene-κN)methyl]-1H-pyrrole-2-propanamidato-

κN1]difluoro-, (T-4)- (CA INDEX NAME)



IT 937803-31-1
RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(as second label; labels binding to reduced cysteine groups of proteins and reducing agent in determination of redox status of proteins)
RN 937803-31-1 CAPLUS
CN Boron, [N-[5-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)pentyl]-5-[[5-(4-methoxyphenyl)-2H-pyrrol-2-ylidene-κN]methyl]-2,4-dimethyl-1H-pyrrole-3-propanamidato-κN1]difluoro-, (T-4)- (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 3 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:329285 CAPLUS Full-text
DOCUMENT NUMBER: 146:358975
TITLE: Preparation of fluoroboron heterocycle-maleimide compound as fluorescent probe
INVENTOR(S): Matsumoto, Takuya; Shoda, Takuji; Urano, Yasuteru; Nagano, Tetsuo
PATENT ASSIGNEE(S): The University of Tokyo, Japan
SOURCE: PCT Int. Appl., 33pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007032363	A1	20070322	WO 2006-JP318104	20060913

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,

GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP,
KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN,
MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS,
RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ,
UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM
PRIORITY APPLN. INFO.: JP 2005-264776 A 20050913
OTHER SOURCE(S): MARPAT 146:358975
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compound I [R1, R2 = H, Q1 with the proviso that both R1 and R2 cannot simultaneously be H; X1, X2 = H, (un)substituted alkyl, (un)substituted alkoxy, etc.; R3, R6 = (un)substituted alkyl; R4, R7 = H, (un)substituted alkyl, carboxyl, etc.; R5, R8 = (un)substituted alkyl, (un)substituted aryl, (un)substituted alkoxycarbonyl, etc.] or salts thereof was prepared For example, reaction of compound II [R = NH2], e.g., prepared from 2-nitrobenzaldehyde in 2 steps, with maleic anhydride followed by treatment with acetic anhydride afforded compound II [R = 1-maleimidyl]. Michael addition of acetone (1 mL) to compound II [R = 1-maleimidyl] (50 μmol) in the presence of L-proline (25 μmol) afforded compound III in 51% yield, which showed a strong fluorescent quantum yield (≥0.6). Of note, compound I is useful for screening of a chemical substance having an applicability as a catalyst in Michael addition reaction.

CC 29-4 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 27, 34, 73

IT Fluorescent indicators
Michael reaction
(preparation of fluoroboron heterocycle-maleimide compound as fluorescent probe)

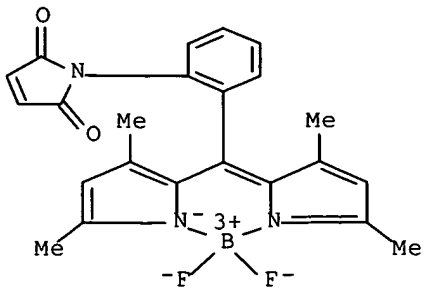
IT 929679-22-1P 929679-25-4P
RL: ARG (Analytical reagent use); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of fluoroboron heterocycle-maleimide compound as fluorescent probe)

IT 929534-11-2DP, Michael addition product with fluoroboron heterocycle-maleimide compound 929534-12-3DP, Michael addition product with fluoroboron heterocycle-maleimide compound 929679-25-4DP, Michael addition product with peptide containing adjacent 2 cysteine residue 929679-26-5P 929679-27-6P 929679-28-7P 929679-29-8P 929679-30-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of fluoroboron heterocycle-maleimide compound as fluorescent probe)

IT 929679-22-1P 929679-25-4P
RL: ARG (Analytical reagent use); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of fluoroboron heterocycle-maleimide compound as fluorescent probe)

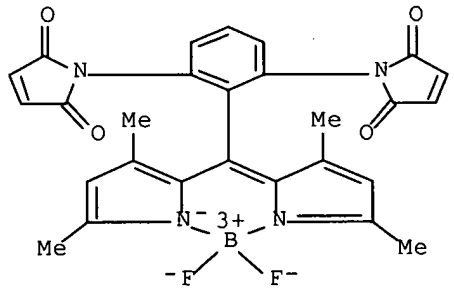
RN 929679-22-1 CAPLUS

CN Boron, [1-[2-[(3,5-dimethyl-1H-pyrrol-2-yl-κN)(3,5-dimethyl-2H-pyrrol-2-ylidene-κN)methyl]phenyl]-1H-pyrrole-2,5-dionato]difluoro-, (T-4)- (CA INDEX NAME)



RN 929679-25-4 CAPLUS

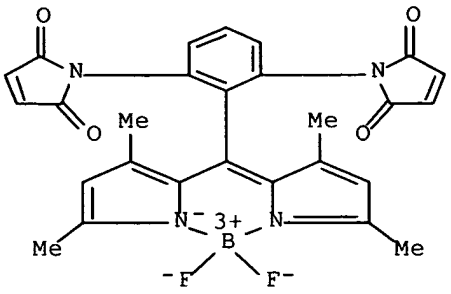
CN Boron, [[1,1'-[2-[(3,5-dimethyl-1H-pyrrol-2-yl-κN)(3,5-dimethyl-2H-pyrrol-2-ylidene-κN)methyl]-1,3-phenylene]bis[1H-pyrrole-2,5-dionato]](1-)]difluoro-, (T-4)- (CA INDEX NAME)



IT 929679-25-4DP, Michael addition product with peptide containing adjacent 2 cysteine residue
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of fluoroboron heterocycle-maleimide compound as fluorescent probe)

RN 929679-25-4 CAPLUS

CN Boron, [[1,1'-[2-[(3,5-dimethyl-1H-pyrrol-2-yl-κN)(3,5-dimethyl-2H-pyrrol-2-ylidene-κN)methyl]-1,3-phenylene]bis[1H-pyrrole-2,5-dionato]](1-)]difluoro-, (T-4)- (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:206414 CAPLUS Full-text
DOCUMENT NUMBER: 146:465146
TITLE: Self-Assembling Light-Harvesting Systems from Synthetically Modified Tobacco Mosaic Virus Coat Proteins
AUTHOR(S): Miller, Rebekah A.; Presley, Andrew D.; Francis, Matthew B.
CORPORATE SOURCE: Department of Chemistry, University of California, Berkeley, CA, 94720-1460, USA
SOURCE: Journal of the American Chemical Society (2007), 129(11), 3104-3109
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new protein-based approach was developed for the construction of light-harvesting systems through self-assembly. The building blocks were prepared by attaching fluorescent chromophores to cysteine residues introduced on tobacco mosaic virus coat protein monomers. When placed under the appropriate buffer conditions, these conjugates could be assembled into stacks of disks or into rods that reached hundreds of nanometers in length. Characterization of the system using fluorescence spectroscopy indicated that efficient energy transfer could be achieved from large nos. of donor chromophores to a single acceptor. Energy transfer probably occurs through direct donor-acceptor interactions, although degenerate donor-to-donor transfer events are also possible. Three-chromophore systems were also prepared to achieve broad spectrum light collection with over 90% overall efficiency. Through the combination of self-organizing biol. structures and synthetic building blocks, a highly tunable new method has emerged for the construction of photovoltaic device components.

CC 52-2 (Electrochemical, Radiational, and Thermal Energy Technology)
Section cross-reference(s): 10, 73

IT 328085-55-8P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Oregon Green 488 maleimide, electron donor; self-assembling light-harvesting systems from synthetically modified tobacco mosaic virus coat proteins)

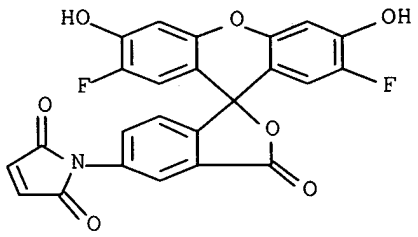
IT 328085-55-8DP, reaction products with tobacco mosaic virus coat proteins 745780-28-3DP, reaction products with tobacco mosaic virus coat proteins 883887-26-1DP, reaction products with tobacco mosaic virus coat

proteins
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(self-assembling light-harvesting systems from synthetically modified tobacco mosaic virus coat proteins)

IT 328085-55-8P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Oregon Green 488 maleimide, electron donor; self-assembling light-harvesting systems from synthetically modified tobacco mosaic virus coat proteins)

RN 328085-55-8 CAPLUS

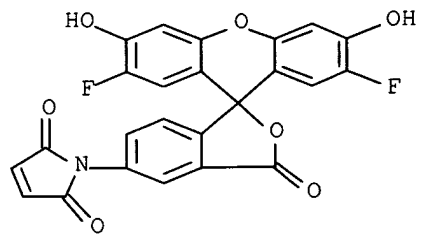
CN 1H-Pyrrole-2,5-dione, 1-(2',7'-difluoro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (CA INDEX NAME)



IT 328085-55-8DP, reaction products with tobacco mosaic virus coat proteins
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(self-assembling light-harvesting systems from synthetically modified tobacco mosaic virus coat proteins)

RN 328085-55-8 CAPLUS

CN 1H-Pyrrole-2,5-dione, 1-(2',7'-difluoro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (CA INDEX NAME)



REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 5 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:73884 CAPLUS Full-text

DOCUMENT NUMBER: 146:420139

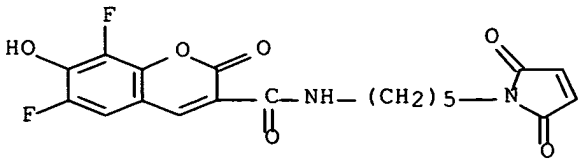
TITLE: A robust method for production of MHC tetramers with small molecule fluorophores

AUTHOR(S): Ramachandiran, Vasanthi; Grigoriev, Vitalii; Lan, Lan; Ravkov, Eugene; Mertens, Suzanne A.; Altman, John D.

CORPORATE SOURCE: Department of Microbiology and Immunology, Emory University School of Medicine, Atlanta, GA, USA
SOURCE: Journal of Immunological Methods (2007), 319(1-2), 13-20
CODEN: JIMMBG; ISSN: 0022-1759
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

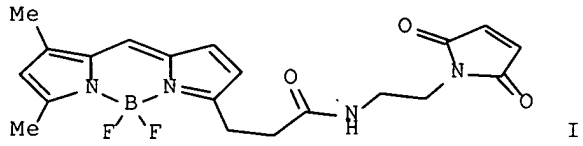
AB Tetramers of major histocompatibility complex mols. (MHC) are now well-established reagents for the detection of antigen-specific T cells by flow cytometry. MHC tetramers are prepared by mixing enzymically biotinylated MHC mols. with com. prepns. of streptavidin, usually conjugated to a fluorescent phycobiliprotein such as phycoerythrin (PE) or allophycocyanin (APC). While data obtained with MHC tetramers prepared with small mol. fluorophores has been reported, considerable lot-to-lot variation among conventional streptavidin conjugates to small mols. prevents routine preparation of such reagents. The authors now report robust preparation of MHC tetramers with small mol. fluorophores, using a recombinant mutant of streptavidin incorporating a C-terminal cysteine in each of the four identical subunits that is conjugated to maleimide derivs. of any of several small mol. fluorophores. These reagents significantly expand the versatility of the MHC tetramer methodol.

CC 15-1 (Immunochemistry)
ST MHC tetramer fluorophore labeling
IT Histocompatibility antigens
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(HLA-A2.1, tetramers, complexes with fluorophore-labeled streptavidin; for detection of T-cells)
IT T cell (lymphocyte)
(fluorophore-labeled streptavidin for MHC tetramer-mediated detection of)
IT Human
(fluorophore-labeled streptavidin for MHC tetramer-mediated detection of T-cells)
IT Human herpesvirus 5
(fluorophore-labeled streptavidin for MHC tetramer-mediated detection of T-cells to)
IT Phosphoproteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(pp65; fluorophore-labeled streptavidin for MHC tetramer-mediated detection of T-cells to)
IT 934216-71-4D, Pacific Blue maleimide, streptavidin conjugates
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(Pacific Blue maleimide; for MHC tetramer-mediated detection of T-cells)
IT 934216-71-4D, Pacific Blue maleimide, streptavidin conjugates
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(Pacific Blue maleimide; for MHC tetramer-mediated detection of T-cells)
RN 934216-71-4 CAPLUS
CN 2H-1-Benzopyran-3-carboxamide, N-[5-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)pentyl]-6,8-difluoro-7-hydroxy-2-oxo- (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:1286954 CAPLUS Full-text
DOCUMENT NUMBER: 146:273726
TITLE: Synthesis and quality control of thiol tagged compound libraries for chemical microarrays
AUTHOR(S): Maier, Sabine; Frank, Michael; Rau, Harald; Lewandrowski, Peter; Uhrig, Rainer; Keil, Oliver; Deppe, Holger; Mueller, Norbert; Vanier, Cecile; Mannsperger, Heiko; Zepter, Siglinde; Junker, Hans-Dieter
CORPORATE SOURCE: Graffinity Pharmaceuticals GmbH, Heidelberg, 69120, Germany
SOURCE: QSAR & Combinatorial Science (2006), 25(11), 1047-1054
CODEN: QCSSAU; ISSN: 1611-020X
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:273726
GI



I

AB A library of N-acyl amino acid amides with pendant thiol moieties is prepared on solid-phase; the purity of the library components is assayed by reaction of samples of thiols with a maleimide-substituted dye, allowing facile anal. of the reaction products by LC-MS. Coupling of a modified trityl-protected mercaptodioxodiazatetraoxaeicosanamine to membranes followed by cleavage of the terminal Fmoc group, coupling with Fmoc-protected amino acids, Fmoc cleavage, coupling with carboxylic acids, and cleavage from the resin membrane provide the product thiols. Addition of a sample of each thiol in acetonitrile-water to a solution of the maleimide-substituted dye I in pH 7.5 phosphate buffer allows the thiol products to be analyzed by LC-MS; excess dye reacts with added 1-octanethiol to generate a comparison peak for LC-MS anal. The extinction coefficient of the dye-maleimide compound removes uncertainty in anal. from variations in the extinction coeffs. of the library compds.; the ratio of the dye-library conjugates to the dye-octanethiol conjugate can be determined, allowing the concentration and purity of library compds. to be

determined as well. The library compds. can be attached to microarrays through their thiol groups; as a result, non-thiol containing byproducts can be removed during immobilization and can be neglected in the purity anal. While LC-MS of the library mixts. includes byproducts that lack thiol groups and are not incorporated into the microarrays, the LC-MS of dye labeled mixts. shows only the thiol-containing products that will be incorporated into the library microarrays.

CC 21-2 (General Organic Chemistry)
Section cross-reference(s): 34, 80

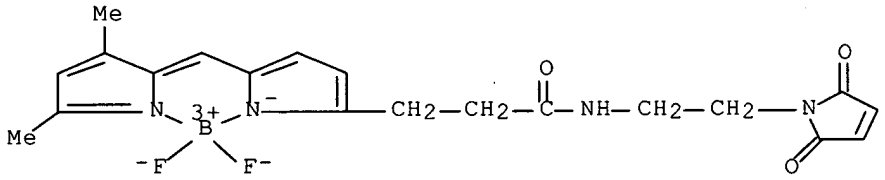
ST acylamino acid amide pendant thiol library prepn analysis; LC MS analysis acylamino acid amide pendant thiol library; mercaptodioxodiazatetraoxaeicosyl acyl amino acid amide prepn quantitation; addn thiol library dye labeled maleimide LC MS analysis

IT 111-88-6, 1-Octanethiol 773859-49-7, BODIPY FL maleimide
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(solid-phase preparation of a microarray combinatorial library of N-acyl amino acid amides with pendant thiol moieties and the use of a maleimide-substituted dye for anal. of the thiol-containing library compds. by LC-MS)

IT 773859-49-7, BODIPY FL maleimide
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(solid-phase preparation of a microarray combinatorial library of N-acyl amino acid amides with pendant thiol moieties and the use of a maleimide-substituted dye for anal. of the thiol-containing library compds. by LC-MS)

RN 773859-49-7 CAPLUS

CN Boron, [N-[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]-5-[(3,5-dimethyl-2H-pyrrol-2-ylidene-κN)methyl]-1H-pyrrole-2-propanamidato-κN1]difluoro-, (T-4)- (CA INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 7 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:1109612 CAPLUS Full-text
DOCUMENT NUMBER: 145:456345
TITLE: Water-soluble fluoro-substituted cyanine dyes, as reactive fluorescence labeling reagents, and precursor 2-methyl-3H-indole derivatives
INVENTOR(S): Cooper, Michael Edward; Gardner, Nicholas John; Laughton, Peter Gordon
PATENT ASSIGNEE(S): Ge Healthcare UK Limited, UK
SOURCE: Brit. UK Pat. Appl., 102pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

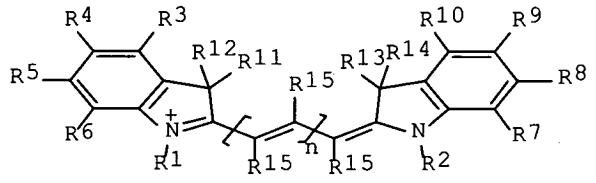
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2425315	A	20061025	GB 2006-7571	20060418
AU 2006238753	A1	20061026	AU 2006-238753	20060418
WO 2006111726	A1	20061026	WO 2006-GB1400	20060418
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
GB 2434150	A	20070718	GB 2007-6473	20060418
US 2006239922	A1	20061026	US 2006-379596	20060421

PRIORITY APPLN. INFO.:

GB 2005-8082	A	20050422
GB 2005-17656	A	20050831
GB 2006-7571	A3	20060418
WO 2006-GB1400	W	20060418

OTHER SOURCE(S): MARPAT 145:456345

GI



I

AB Disclosed are cyanine dyes that are useful for labeling and detecting biol. and other materials. The dyes are of formula I: in which the substituents are as defined in claim 1 and, in particular, at least one of groups R, R is -L-M or -L-P, where L is a linking group, M is a target bonding group and P is a conjugated component, and at least one of groups R, R comprises F. The use of cyanine dyes substituted by fluorine and having addnl. substitution with three or more sulfonic acid groups for labeling biol. target mols. results in a labeled product in which there is reduced dye-dye aggregation and improved photostability, compared with cyanine dyes having no such substitutions. The dyes of the present invention are particularly useful in assays involving fluorescence detection where continual or repeated excitation is a requirement, for example in kinetic studies, or in microarray analyses where microarray slides may need to be reanalyzed over a period of days. Also disclosed are precursor 2-methyl-indolinium derivs. as defined in claim 46, as well as related cyanine dyes and 2-methyl-indolinium derivs. as defined in claims 35, 53 and 56, and 4,5,6,7-tetrafluoro-2,3-dimethyl-3H-indoles with either a 5-carboxypentyl or 4-sulfobutyl substituent in the 3-position.

CC 41-11 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic

Sensitizers)
Section cross-reference(s): 9
ST cyanine dye fluorescence labeling detection; methylindole precursor fluorescence labeling dye
IT Antibodies and Immunoglobulins
RL: MSC (Miscellaneous)
(conjugation with; manufacture of water-soluble fluoro-substituted cyanine dyes
useful for reactive fluorescence labeling reagents, and precursor 2-Me-3H-indole derivs.)
IT Cyanine dyes
Fluorescent indicators
(manufacture of water-soluble fluoro-substituted cyanine dyes useful for reactive fluorescence labeling reagents, and precursor 2-Me-3H-indole derivs.)
IT 252358-62-6P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(dye intermediate; manufacture of water-soluble fluoro-substituted cyanine dyes
useful for reactive fluorescence labeling reagents, and precursor 2-Me-3H-indole derivs.)
IT 913198-38-6P 913198-39-7P 913198-40-0P 913198-41-1P 913198-42-2P
913198-43-3P 913198-44-4P 913198-45-5P 913198-46-6P 913198-47-7P
913198-48-8P 913198-49-9P 913198-50-2P 913198-51-3P 913198-52-4P
913198-53-5P 913198-54-6P 913198-55-7P 913198-56-8P 913198-57-9P
913198-58-0P 913198-59-1P
RL: IMF (Industrial manufacture); PRP (Properties); RGT (Reagent); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(dye; manufacture of water-soluble fluoro-substituted cyanine dyes useful for
reactive fluorescence labeling reagents, and precursor 2-Me-3H-indole derivs.)
IT 913198-63-7P 913198-64-8P 913198-90-0P 913198-91-1P
RL: IMF (Industrial manufacture); PRP (Properties); RGT (Reagent); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(manufacture of water-soluble fluoro-substituted cyanine dyes useful for reactive fluorescence labeling reagents, and precursor 2-Me-3H-indole derivs.)
IT 1150-36-3P 88575-32-0P, p-(Trifluoromethylthio)phenylhydrazine
407627-51-4P 688339-30-2P, 5-Methyl-6-oxoheptane-1-sulfonic acid
688339-34-6P 851528-20-6P, Sodium 5-(ethoxycarbonyl)-5-methyl-6-oxoheptane-1-sulfonate 913198-60-4P 913198-61-5P 913198-62-6P
913198-66-0P 913198-67-1P 913198-69-3P 913198-70-6P 913198-71-7P
913198-73-9P 913198-74-0P 913198-75-1P 913198-76-2P 913198-77-3P
913198-78-4P 913198-79-5P 913198-80-8P 913198-81-9P 913198-82-0P
913198-83-1P 913198-84-2P 913198-85-3P 913198-86-4P 913198-87-5P
913198-88-6P 913198-89-7P 913198-92-2P 913198-93-3P 913198-94-4P
913198-95-5P 913198-96-6P 913198-97-7P 913198-98-8P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(manufacture of water-soluble fluoro-substituted cyanine dyes useful for reactive fluorescence labeling reagents, and precursor 2-Me-3H-indole derivs.)
IT 98-71-5, 4-Hydrazinobenzenesulfonic acid 313-72-4, Octafluoronaphthalene
368-90-1, 4-(Trifluoromethyl)phenyl hydrazine 372-16-7,
4-(Trifluoromethylthio)aniline 563-80-4, 3-Methyl-2-butanone 609-14-3,
Ethyl 2-methylacetoacetate 886-35-1, 3,5-Bis(trifluoromethyl)phenyl

hydrazine 1497-49-0 1633-83-6, 1,4-Butanesultone 4224-70-8, 6-Bromohexanoic acid 5580-80-3, 2,3,4,5-Tetrafluoroaniline 7632-00-0, Sodium nitrite 7803-57-8, Hydrazine hydrate 22697-22-9 41638-17-9, Trimethoxypropene 99183-34-3 123071-42-1, Malonaldehyde bisphenylimine monohydrochloride 134272-63-2 146368-08-3 207683-26-9 407627-97-8, 7-Methyl-8-oxononanoic acid 502496-23-3 502496-27-7 851588-34-6 913198-65-9 913198-68-2 913198-72-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(manufacture of water-soluble fluoro-substituted cyanine dyes useful for reactive fluorescence labeling reagents, and precursor 2-Me-3H-indole derivs.)

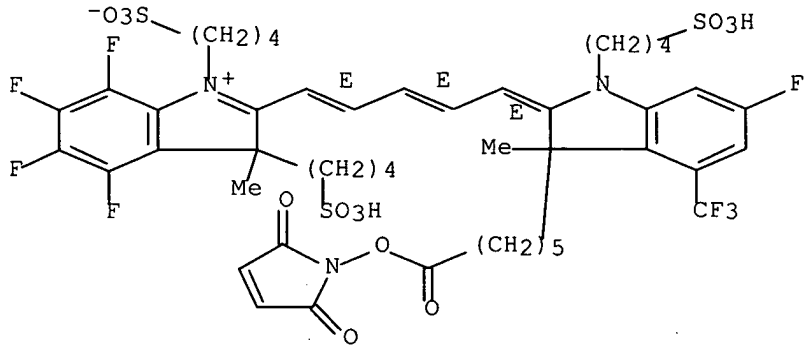
IT 1333-82-0, Chromium trioxide
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidant; manufacture of water-soluble fluoro-substituted cyanine dyes useful for reactive fluorescence labeling reagents, and precursor 2-Me-3H-indole derivs.)

IT 913198-91-1P
RL: IMF (Industrial manufacture); PRP (Properties); RGT (Reagent); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(manufacture of water-soluble fluoro-substituted cyanine dyes useful for reactive fluorescence labeling reagents, and precursor 2-Me-3H-indole derivs.)

RN 913198-91-1 CAPLUS

CN 3H-Indolium, 2-[(1E,3E,5E)-5-[3-[6-[(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)oxy]-6-oxohexyl]-6-fluoro-1,3-dihydro-3-methyl-1-(4-sulfobutyl)-4-(trifluoromethyl)-2H-indol-2-ylidene]-1,3-pentadienyl]-4,5,6,7-tetrafluoro-3-methyl-1,3-bis(4-sulfobutyl)-, inner salt (9CI) (CA INDEX NAME)

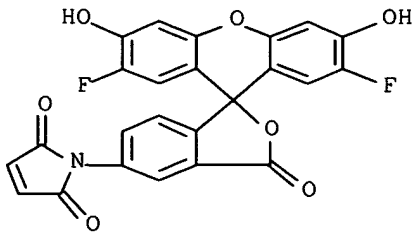
Double bond geometry as shown.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 8 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:1007503 CAPLUS Full-text
DOCUMENT NUMBER: 146:3359
TITLE: Spatially and temporally synchronized atomic force and total internal reflection fluorescence microscopy for imaging and manipulating cells and biomolecules
AUTHOR(S): Kellermayer, Miklos S. Z.; Karsai, Arpad; Kengyel, Andras; Nagy, Attila; Bianco, Pasquale; Huber, Tamas;

Kulcsar, Agnes; Niedetzky, Csaba; Proksch, Roger; Grama, Laszlo
CORPORATE SOURCE: Department of Biophysics, Faculty of Medicine, University of Pecs, Pecs, H-7624, Hung.
SOURCE: Biophysical Journal (2006), 91(7), 2665-2677
CODEN: BIOJAU; ISSN: 0006-3495
PUBLISHER: Biophysical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The atomic force microscope is a high-resolution scanning-probe instrument which has become an important tool for cellular and mol. biophysics in recent years but lacks the time resolution and functional specificities offered by fluorescence microscopic techniques. To exploit the advantages of both methods, here the authors developed a spatially and temporally synchronized total internal reflection fluorescence and atomic force microscope system. The instrument, which the authors hereby call STIRF-AFM, is a stage-scanning device in which the mech. and optical axes are coaligned to achieve spatial synchrony. At each point of the scan the sample topog. (atomic force microscope) and fluorescence (photon count or intensity) information are simultaneously recorded. The tool was tested and validated on various cellular (monolayer cells in which actin filaments and intermediate filaments were fluorescently labeled) and biomol. (actin filaments and titin mols.) systems. The authors demonstrate that with the technique, correlated sample topog. and fluorescence images can be recorded, soft biomol. systems can be mech. manipulated in a targeted fashion, and the fluorescence of mech. stretched titin can be followed with high temporal resolution
CC 9-4 (Biochemical Methods)
Section cross-reference(s): 13
IT Atomic force microscopy
Cell
Fluorescent indicators
HeLa cell
Human
Laser fluorometry
Laser induced fluorescence
Single molecule detection
(spatially and temporally synchronized atomic force and total internal reflection fluorescence microscopy for imaging and manipulating cells and biomols.)
IT 17466-45-4D, Phalloidin, TRITC-conjugate 27072-45-3D, Fluorescein isothiocyanate, secondary IgG conjugates 107347-53-5D, TRITC, phalloidin-conjugate 328085-55-8, Oregon Green 488 maleimide 669720-16-5
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(spatially and temporally synchronized atomic force and total internal reflection fluorescence microscopy for imaging and manipulating cells and biomols.)
IT 328085-55-8, Oregon Green 488 maleimide
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(spatially and temporally synchronized atomic force and total internal reflection fluorescence microscopy for imaging and manipulating cells and biomols.)
RN 328085-55-8 CAPLUS
CN 1H-Pyrrole-2,5-dione, 1-(2',7'-difluoro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (CA INDEX NAME)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 9 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:990751 CAPLUS Full-text
DOCUMENT NUMBER: 146:3355
TITLE: Evaluation of disulfide reduction during receptor-mediated endocytosis by using FRET imaging
AUTHOR(S): Yang, Jun; Chen, Hongtao; Vlahov, Iontcho R.; Cheng, Ji-Xin; Low, Philip S.
CORPORATE SOURCE: Dep. Chem., Purdue Univ., West Lafayette, IN, 47907, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2006), 103(37), 13872-13877
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

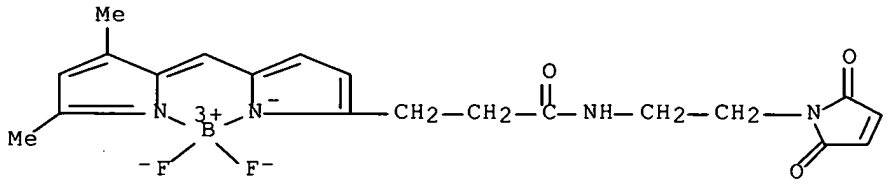
AB Despite functional evidence for disulfide bond-reducing activity in endosomal compartments, the mechanistic details pertaining to such process (e.g., kinetics and sites of disulfide reduction) remain largely controversial. To address these questions directly, the authors have synthesized a previously uncharacterized fluorescent folate conjugate, folate-(BODIPY FL)-SS-rhodamine (folate-FRET), that changes fluorescence from red to green upon disulfide bond reduction Using this construct, the authors have observed that disulfide reduction: (i) occurs with a half-time of 6 h after folate-FRET endocytosis, (ii) begins in endosomes and does not depend significantly on redox machinery located on the cell surface or within the lysosome or the Golgi apparatus, (iii) occurs independently of endocytic vesicle trafficking along microtubules, and (iv) yields products that are subsequently sorted into distinct endosomes and trafficked in different directions. Finally, colocalization of folate and transferrin receptors suggest that conclusions derived from this study may apply to other endocytic pathways.

CC 9-4 (Biochemical Methods)
Section cross-reference(s): 28

IT Disulfide group
Endosome
Fluorescence
Fluorescence resonance energy transfer
Fluorescent indicators
Fluorometry
Human
(evaluation of disulfide bond reduction during receptor-mediated endocytosis by using FRET imaging)

IT 146616-66-2 386229-71-6 773859-49-7, BODIPY FL maleimide
RL: RCT (Reactant); RACT (Reactant or reagent)
(evaluation of disulfide bond reduction during receptor-mediated

endocytosis by using FRET imaging)
IT 773859-49-7, BODIPY FL maleimide
RL: RCT (Reactant); RACT (Reactant or reagent)
(evaluation of disulfide bond reduction during receptor-mediated endocytosis by using FRET imaging)
RN 773859-49-7 CAPLUS
CN Boron, [N-[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]-5-[(3,5-dimethyl-2H-pyrrol-2-ylidene-κN)methyl]-1H-pyrrole-2-propanamidato-κN1]difluoro-, (T-4)- (CA INDEX NAME)



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 10 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:646539 CAPLUS Full-text
DOCUMENT NUMBER: 145:173868
TITLE: Semitelechelic HPMA Copolymers Functionalized with Triphenylphosphonium as Drug Carriers for Membrane Transduction and Mitochondrial Localization
AUTHOR(S): Callahan, Jon; Kopecek, Jindrich
CORPORATE SOURCE: Department of Bioengineering, University of Utah, Salt Lake City, UT, 84112, USA
SOURCE: Biomacromolecules (2006), 7(8), 2347-2356
CODEN: BOMAF6; ISSN: 1525-7797
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Semitelechelic HPMA (N-(2-hydroxypropyl)methacrylamide) copolymers possessing a single terminal lipophilic triphenylphosphonium (TPP) cation and fluorescent labels were synthesized to determine how the attached cation affected cellular uptake and intracellular trafficking. In vitro mitochondrial uptake fluorescence quenching assays using isolated mouse liver mitochondria indicated that only lower mol. weight (<5 kDa) BODIPY FL-labeled TPP-semitelechelic HPMA copolymers exhibited significant organelle localization or uptake. In vitro cellular uptake and intracellular trafficking was evaluated using cultured human ovarian carcinoma cells. Cells incubated with all types of TPP copolymers used in the study appeared to internalize the polymer by endocytosis only, and all of the internalized copolymer was confined to the lysosomal compartment after 24 h. Endocytic uptake of the TPP-HPMA copolymer conjugates was rapid, suggesting that they were internalized by adsorptive endocytosis, rather than fluid-phase pinocytosis. Low-mol. weight (<5 kDa) and high-mol. weight (>5 kDa) semitelechelic copolymers, microinjected into cultured cells indicated that the TPP moiety did not significantly localize the polymers to mitochondria.

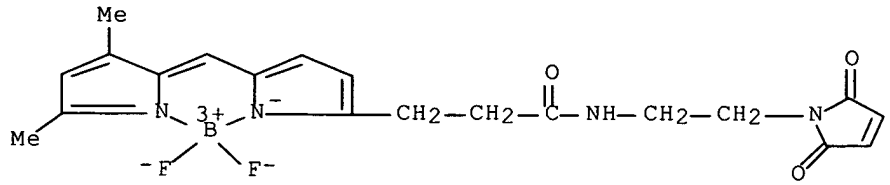
CC 63-5 (Pharmaceuticals)
IT 507-09-5, Thiolacetic acid, reactions 603-35-0, Triphenylphosphine, reactions 5162-44-7, 4-Bromo-1-butene 57950-79-5 220524-70-9 773859-49-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(semitelechelic HPMA copolymers functionalized with triphenylphosphonium as drug carriers for membrane transduction and mitochondrial localization)

IT 773859-49-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(semitelechelic HPMA copolymers functionalized with triphenylphosphonium as drug carriers for membrane transduction and mitochondrial localization)

RN 773859-49-7 CAPLUS

CN Boron, [N-[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]-5-[(3,5-dimethyl-2H-pyrrol-2-ylidene-κN)methyl]-1H-pyrrole-2-propanamidato-κN1]difluoro-, (T-4)- (CA INDEX NAME)



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 11 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:365240 CAPLUS Full-text
DOCUMENT NUMBER: 144:412505
TITLE: Benzimidazole or indole amides as inhibitors of pin1 and their preparation, pharmaceutical compositions, and use for treatment of diseases associated with abnormal cell growth
INVENTOR(S): Do, Quyen-Quyen Thuy; Guo, Chuangxing; Humphries, Paul Stuart; Marakovits, Joseph Timothy; Dong, Liming; Hou, Xinjun; Johnson, Mary Catherine
PATENT ASSIGNEE(S): Pfizer, Inc., USA
SOURCE: PCT Int. Appl., 396 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006040646	A1	20060420	WO 2005-IB3019	20051003

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,

GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-619211P P 20041014

OTHER SOURCE(S): MARPAT 144:412505

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to compds. of the formula I and to pharmaceutically acceptable salts and solvates thereof, wherein the variables are defined herein. The invention also relates to methods of treating abnormal cell growth in mammals by administering the compds. of formula I and to pharmaceutical compns. for treating such disorders that contain the compds. of formula I. The invention also relates to methods of preparing the compds. of formula I. Compds. of formula I wherein Q, Q1, Q2, and Q3 are independently N, CH2 or CH, where not more than two of the Qs are N; T is CH or N; T1 is O, NH or NMe; X is NH, O, CH=, or NR'; R' is (un)substiuted alkyl; Y is CO, CH2, or CONH and derivs.; Z is H or (un)substiuted alkyl; XY and X can form a heterocyclic ring or X and Y can form a heterocyclic ring; R and V are independently H, halo, alkyl, halogenated alkyl, alkoxy, OH, NH2, CN; R1 is (un)substituted (hetero)aryl, (un)substituted aryloxy, (un)substituted arylsulfanyl, (un)substituted arylvinyl or (un)substituted arylalkyl(amino), etc.; R3 is CO2H, tetrazole, CO2CHR4OCOR4 or CONH2 and derivs.; R4 is H or alkyl; and their pharmaceutically acceptable salts and solvates are claimed in this invention. Example compound II was prepared by substitution of compound II with benzoxazole-2-thiol followed by hydrolysis at the ester. Addnl. 1400 example compds. were prepared in this invention. All invention compds. were evaluated for their pin1 inhibitory activity. Example compound II showed 10% inhibition at 1 μM and 73% inhibition at 10 μM concentration Most of the invention compds. showed good inhibitory activity at 10 μM concentration

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

IT Biomarkers
(modifiers; preparation of benzimidazole or indole amides as inhibitors of pin1 useful for treatment of diseases associated with abnormal cell growth)

IT

884033-47-0P	884033-48-1P	884033-49-2P	884033-51-6P	884033-52-7P
884033-54-9P	884033-56-1P	884033-57-2P	884033-58-3P	884033-59-4P
884033-60-7P	884033-61-8P	884033-63-0P	884033-64-1P	884033-65-2P
884033-68-5P	884033-70-9P	884033-71-0P	884033-72-1P	884033-75-4P
884033-77-6P	884033-79-8P	884033-80-1P	884033-81-2P	884033-82-3P
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884036-73-1P 884036-74-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzimidazole or indole amides as inhibitors of pin1 useful for treatment of diseases associated with abnormal cell growth)

IT 884041-43-4P 884041-44-5P 884041-45-6P 884041-46-7P 884041-47-8P
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884043-76-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzimidazole or indole amides as inhibitors of pin1 useful for treatment of diseases associated with abnormal cell growth)

IT 884034-44-0P 884035-71-6P 884042-58-4P
884042-69-7P

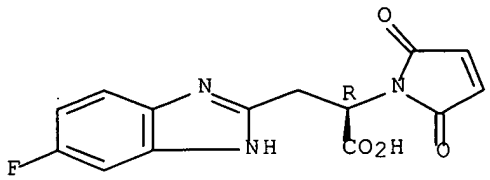
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzimidazole or indole amides as inhibitors of pin1 useful for treatment of diseases associated with abnormal cell growth)

RN 884034-44-0 CAPLUS

CN 1H-Benzimidazole-2-propanoic acid, α-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-5-fluoro-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



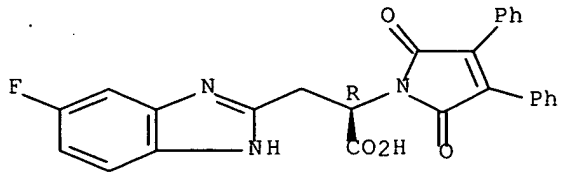
RN 884035-71-6 CAPLUS

CN 1H-Benzimidazole-2-propanoic acid, α-(2,5-dihydro-2,5-dioxo-3,4-diphenyl-1H-pyrrol-1-yl)-5-fluoro-, (αR)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

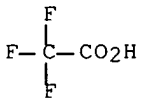
CRN 884035-70-5
CMF C26 H18 F N3 O4

Absolute stereochemistry.



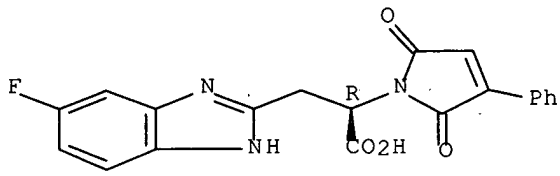
CM 2

CRN 76-05-1
CMF C2 H F3 O2



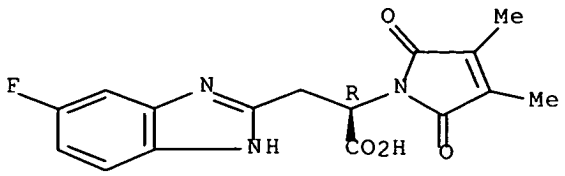
RN 884042-58-4 CAPLUS
CN 1H-Benzimidazole-2-propanoic acid, α-(2,5-dihydro-2,5-dioxo-3-phenyl-1H-pyrrol-1-yl)-5-fluoro-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 884042-69-7 CAPLUS
CN 1H-Benzimidazole-2-propanoic acid, α-(2,5-dihydro-3,4-dimethyl-2,5-dioxo-1H-pyrrol-1-yl)-5-fluoro-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 12 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:203247 CAPLUS Full-text
DOCUMENT NUMBER: 144:428162
TITLE: Fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture
AUTHOR(S): Krahn, Katy Nash; Bouten, Carlijn V. C.; Van Tuijl, Sjoerd; Van Zandvoort, Marc A. M. J.; Merkx, Maarten
CORPORATE SOURCE: Laboratory for Cell and Tissue Engineering, Department of Biomedical Engineering, Eindhoven University of Technology, Eindhoven, 5600 MB, Neth.
SOURCE: Analytical Biochemistry (2006), 350(2), 177-185
CODEN: ANBCA2; ISSN: 0003-2697
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Visualization of the formation and orientation of collagen fibers in tissue engineering expts. is crucial for understanding the factors that determine the mech. properties of tissues. In this study, collagen-specific fluorescent probes were developed using a new approach that takes advantage of the inherent specificity of collagen binding protein domains present in bacterial adhesion proteins (CNA35) and integrins (GST-α1I). Both collagen binding domains were obtained as fusion proteins from an Escherichia coli expression system and fluorescently labeled using either amine-reactive succinimide (CNA35) or cysteine-reactive maleimide (GST-α1I) dyes. Solid-phase binding assays showed that both protein-based probes are much more specific than dichlorotriazinyl aminofluorescein (DTAF), a fluorescent dye that is currently used to track collagen formation in tissue engineering expts. The CNA35 probe showed a higher affinity for human collagen type I than did the GST-α1I probe (apparent Kd values of 0.5 and 50 μM, resp.) and showed very little cross-reactivity with noncollagenous extracellular matrix proteins. The CNA35 probe was also superior to both GST-α1I and DTAF in visualizing the formation of collagen fibers around live human venous saphena cells. Immunohistol. expts. on rat tissue showed colocalization of the CNA35 probe with collagen type I and type III antibodies. The fluorescent probes described here have important advantages over existing methods for visualization of collagen, in particular for monitoring the formation of collagen in live tissue cultures over prolonged time periods.

CC 9-4 (Biochemical Methods)
ST collagen visualization fluorescently labeled binding protein tissue
IT Proteins
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(CNA35, fluorescently labeled; fluorescently labeled collagen binding proteins allow specific visualization of collagen in

tissues and live cell culture)

IT Proteins
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(collagen-binding; fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture)

IT Imaging
Imaging agents
(fluorescent; fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture)

IT Affinity
Animal tissue
Animal tissue culture
Confocal laser scanning microscopy
Dissociation constant
Fluorescence
Fluorescence microscopy
Fluorescent indicators
Fluorometry
Human
Molecular association
Molecular recognition
Tissue engineering
(fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture)

IT Collagen fibers
Collagens, analysis
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture)

IT Spinal column
(intervertebral disk; fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture)

IT Muscle
Tendon
(muscle-tendon junction; fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture)

IT Vein
(saphenous; fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture)

IT Collagens, analysis
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(type I; fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture)

IT Collagens, analysis
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(type II; fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture)

IT Collagens, analysis
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical

study); BIOL (Biological study)
(type III; fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture)

IT Collagens, analysis
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(type IV; fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture)

IT Collagens, analysis
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(type V; fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture)

IT Collagens, analysis
RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(type VI; fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture)

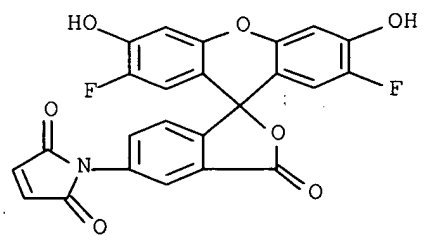
IT Integrins
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(α1, I domain, fusion protein with glutathione transferase, fluorescently labeled; fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture)

IT 50812-37-8D, Glutathione S-transferase, fusion protein with integrin α1 I domain, fluorescently labeled 178623-13-7D, reaction products with protein CNA35 198139-51-4D, Oregon Green 488 carboxylic acid succinimidyl ester, reaction products with protein CNA35 328085-55-8D, Oregon Green 488 maleimide, reaction products with glutathione transferase-integrin α1 I domain fusion protein
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture)

IT 328085-55-8D, Oregon Green 488 maleimide, reaction products with glutathione transferase-integrin α1 I domain fusion protein
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(fluorescently labeled collagen binding proteins allow specific visualization of collagen in tissues and live cell culture)

RN 328085-55-8 CAPLUS

CN 1H-Pyrrole-2,5-dione, 1-(2',7'-difluoro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (CA INDEX NAME)



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 13 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:94604 CAPLUS Full-text
DOCUMENT NUMBER: 144:346168
TITLE: Specific and Stable Fluorescence Labeling of Histidine-Tagged Proteins for Dissecting Multi-Protein Complex Formation
AUTHOR(S): Lata, Suman; Gavutis, Martynas; Tampe, Robert; Piehler, Jacob
CORPORATE SOURCE: Institut fuer Biochemie, Johann Wolfgang Goethe-University, Frankfurt am Main, D-60439, Germany
SOURCE: Journal of the American Chemical Society (2006), 128(7), 2365-2372
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:346168

AB Labeling of proteins with fluorescent dyes offers powerful means for monitoring protein interactions in vitro and in live cells. Only a few techniques for noncovalent fluorescence labeling with well-defined localization of the attached dye are currently available. Here, the authors present an efficient method for site-specific and stable noncovalent fluorescence labeling of histidine-tagged proteins. Different fluorophores were conjugated to a chemical recognition unit bearing three NTA moieties (tris-NTA). In contrast to the transient binding of conventional mono-NTA, the multivalent interaction of tris-NTA conjugated fluorophores with oligohistidine-tagged proteins resulted in complex lifetimes of more than an hour. The high selectivity of tris-NTA toward cumulated histidines enabled selective labeling of proteins in cell lysates and on the surface of live cells. Fluorescence labeling by tris-NTA conjugates was applied for the anal. of a ternary protein complex in solution and on surfaces. Formation of the complex and its stoichiometry was studied by anal. size exclusion chromatog. and fluorescence quenching. The individual interactions were dissected on solid supports by using simultaneous mass-sensitive and multicolor fluorescence detection. Using these techniques, formation of a 1:1:1 stoichiometry by independent interactions of the receptor subunits with the ligand was shown. The incorporation of transition metal ions into the labeled proteins upon labeling with tris-NTA fluorophore conjugates provided an addnl. sensitive spectroscopic reporter for detecting and monitoring protein-protein interactions in real time. A broad application of these fluorescence conjugates for protein interaction anal. can be envisaged.

CC 9-5 (Biochemical Methods)
Section cross-reference(s): 2, 15, 28
ST stable fluorescence labeling histidine tagged protein multiprotein complex
IT Proteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(complexes; specific and stable fluorescence labeling of histidine-tagged proteins for dissecting multi-protein complex formation)
IT Transition metals, biological studies
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(ions; specific and stable fluorescence labeling of

histidine-tagged proteins for dissecting multi-protein complex formation in relation to transition metal ion binding)

IT Proteins
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(labeled, oligohistidine-tagged; specific and stable fluorescence labeling of histidine-tagged proteins for dissecting multi-protein complex formation)

IT Fluorescence
Fluorescence quenching
Fluorescent indicators
Fluorometry
Molecular association
Molecular recognition
Size-exclusion chromatography
Stoichiometry
(specific and stable fluorescence labeling of histidine-tagged proteins for dissecting multi-protein complex formation)

IT Interferon receptors
RL: BUU (Biological use, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); BIOL (Biological study); PROC (Process); USES (Uses)
(α/β-interferon, 2, oligohistidine-tagged, conjugates with fluorophores; specific and stable fluorescence labeling of histidine-tagged proteins for dissecting multi-protein complex formation)

IT Interferons
RL: BUU (Biological use, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); BIOL (Biological study); PROC (Process); USES (Uses)
(α2, conjugates with fluorophores; specific and stable fluorescence labeling of histidine-tagged proteins for dissecting multi-protein complex formation)

IT Interferons
RL: BUU (Biological use, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); BIOL (Biological study); PROC (Process); USES (Uses)
(β, conjugates with fluorophores; specific and stable fluorescence labeling of histidine-tagged proteins for dissecting multi-protein complex formation)

IT 26062-48-6D, Poly-L-histidine, oligomers, -tagged proteins 26854-81-9D, oligomers, -tagged proteins
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(specific and stable fluorescence labeling of histidine-tagged proteins for dissecting multi-protein complex formation)

IT 198139-51-4D, Oregon Green 488 carboxylic acid succinimidyl ester, oligohistidine-tagged interferon α/β receptor conjugates
247144-99-6D, Alexa Fluor 488, interferon α2 conjugates
328085-55-8D, Oregon Green 488 maleimide, interferon α2 conjugates
RL: BUU (Biological use, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); BIOL (Biological study); PROC (Process); USES (Uses)
(specific and stable fluorescence labeling of histidine-tagged proteins for dissecting multi-protein complex formation)

IT 875295-93-5P 881178-44-5P 881178-45-6P 881178-50-3P 881178-51-4P
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(specific and stable fluorescence labeling of histidine-tagged proteins for dissecting multi-protein complex formation)

IT 108-55-4, Glutaric anhydride 5292-43-3, tert-Butyl bromoacetate 80165-23-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(specific and stable fluorescence labeling of histidine-tagged proteins for dissecting multi-protein complex formation)

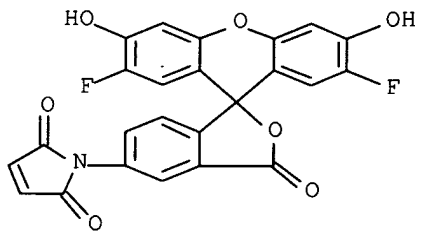
IT 295-37-4P, 1,4,8,11-Tetraazacyclotetradecane 6404-29-1P 63628-63-7P 113231-05-3P 205379-07-3P 205379-08-4P 206265-98-7P 862778-54-9P 862778-55-0P 862778-56-1P 862778-57-2P 862778-60-7P 881178-41-2P 881178-42-3P 881178-43-4P 881178-46-7P 881178-48-9P 881178-49-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(specific and stable fluorescence labeling of histidine-tagged proteins for dissecting multi-protein complex formation)

IT 7440-02-0, Nickel, biological studies
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(specific and stable fluorescence labeling of histidine-tagged proteins for dissecting multi-protein complex formation in relation to transition metal ion binding)

IT 328085-55-8D, Oregon Green 488 maleimide, interferon α2 conjugates
RL: BUU (Biological use, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); BIOL (Biological study); PROC (Process); USES (Uses)
(specific and stable fluorescence labeling of histidine-tagged proteins for dissecting multi-protein complex formation)

RN 328085-55-8 CAPLUS

CN 1H-Pyrrole-2,5-dione, 1-(2',7'-difluoro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 14 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1132015 CAPLUS Full-text
DOCUMENT NUMBER: 144:47481
TITLE: Real-time measurement of solute partitioning to lipid

monolayers

AUTHOR(S): Momsen, W. E.; Mizuno, N. K.; Lowe, M. E.; Brockman, H. L.

CORPORATE SOURCE: The Hormel Institute, University of Minnesota, Austin, MN, 55912, USA

SOURCE: Analytical Biochemistry (2005), 346(1), 139-149
CODEN: ANBCA2; ISSN: 0003-2697

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The interaction of a peripheral protein with a lipid-water interface can show a pronounced dependence on the composition and two-dimensional packing d. of the lipids that comprise the interface. The authors report a novel optical method for measuring the adsorption of macromols., such as proteins and nucleic acids, and smaller solutes, such as drugs, to lipid monolayers at the gas-liquid interface. Using fluorescence emission from proteins and a small mol., the authors demonstrate that the emissions from these solutes when in the aqueous phase and when associated with the monolayer can be temporally separated Such separation allows measurement of the extent of solute adsorption, spectral characterization of the adsorbed solute, and characterization of lipid organization using adsorption kinetics. The method does not require, but is compatible with, the solute having different spectral properties in the bulk and surface phases. Indeed, if optical signals from adsorbed and soluble solute are the same or their relation is known, absolute surface excess of adsorbed solute can be calculated without independent calibration. With appropriate instrumental configuration, the method should be adaptable for screening solutes for interaction with planar monolayers having both well-defined composition and adjustable lipid packing d.

CC 9-5 (Biochemical Methods)

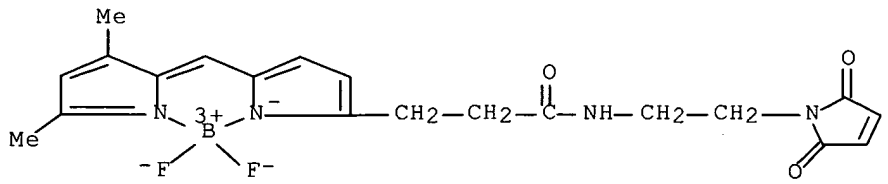
IT Adsorption
Fluorescence
Fluorescent indicators
Fluorometry
Partition
Solutes
(real-time measurement of solute partitioning to lipid monolayers)

IT 55126-92-6, Lipase cofactor 773859-49-7, BODIPY FL-N-(2-aminoethyl)maleimide
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); PROC (Process)
(real-time measurement of solute partitioning to lipid monolayers)

IT 773859-49-7, BODIPY FL-N-(2-aminoethyl)maleimide
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); PROC (Process)
(real-time measurement of solute partitioning to lipid monolayers)

RN 773859-49-7 CAPLUS

CN Boron, [N-[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]-5-[(3,5-dimethyl-2H-pyrrol-2-ylidene-κN)methyl]-1H-pyrrole-2-propanamidato-κN1]difluoro-, (T-4)- (CA INDEX NAME)



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 15 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:463952 CAPLUS Full-text
DOCUMENT NUMBER: 143:168946
TITLE: General, high-affinity approach for the synthesis of fluorophore appended protein nanoparticle assemblies
AUTHOR(S): Sandros, Marinella G.; Gao, De; Gokdemir, Cagil; Benson, David E.
CORPORATE SOURCE: Department of Chemistry, Wayne State University, Detroit, MI, 48202, USA
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2005), (22), 2832-2834
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Metallothionein fusion proteins allow for site-specific, orthogonal functionalization of proteins to a variety of nanoparticles.

CC 9-5 (Biochemical Methods)
Section cross-reference(s): 6

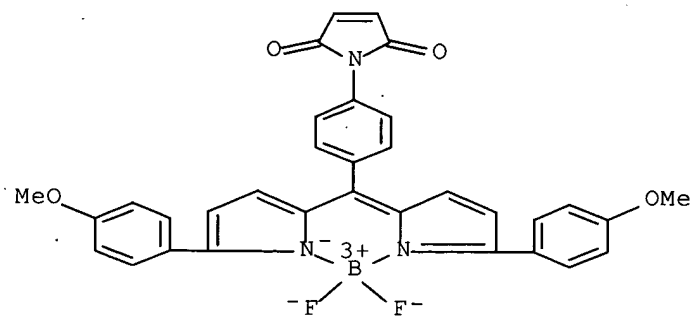
IT Fluorescent indicators
Fluorometry
(general, high-affinity approach for synthesis of fluorophore appended protein nanoparticle assemblies)

IT 632334-55-5, BODIPY 577/618 maleimide
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(BODIPY 577/618 maleimide; general, high-affinity approach for synthesis of fluorophore appended protein nanoparticle assemblies)

IT 632334-55-5, BODIPY 577/618 maleimide
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(BODIPY 577/618 maleimide; general, high-affinity approach for synthesis of fluorophore appended protein nanoparticle assemblies)

RN 632334-55-5 CAPLUS

CN Boron, difluoro[1-[4-[[5-(4-methoxyphenyl)-1H-pyrrol-2-yl-κN][5-(4-methoxyphenyl)-2H-pyrrol-2-ylidene-κN]methyl]phenyl]-1H-pyrrole-2,5-dionato]-, (T-4)- (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 16 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:34864 CAPLUS Full-text
DOCUMENT NUMBER: 142:129778
TITLE: Analysis and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins
INVENTOR(S): Burkart, Michael D.; Laclair, James J.
PATENT ASSIGNEE(S): The Regents of the University of California, USA
SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005003307	A2	20050113	WO 2004-US19568	20040617
WO 2005003307	A3	20060908		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2006216775	A1	20060928	US 2005-561108	20051215

PRIORITY APPLN. INFO.: US 2003-479344P P 20030617
WO 2004-US19568 W 20040617

OTHER SOURCE(S): CASREACT 142:129778

AB This invention generally relates to methods and compns. for identifying biosynthetic enzymes involved in secondary metabolic biosynthesis or other proteins of interest, and in particular relating to fatty acid synthases (FAS), polyketide synthases (PKS), and non-ribosomal peptide synthases (NRPS). The compns. further provide microarray anal. and provide a viable screen for genetic and proteomic events in natural and engineered systems. Using recombinant DNA and mol. genetic methods, carrier protein domains can be cloned in fusion with any protein of interest. The resulting fusion system thereby allows the methods and compns. of the present invention to be extended to the study of any protein of interest. A method for detecting a protein of interest comprises contacting a coenzyme with a synthetic appendage label, contacting a carrier protein domain with the protein of interest to form a carrier protein (CP) domain-protein of interest (POI) complex, contacting the CP-POI complex with the labeled coenzyme, and detecting the labeled carrier protein domain to detect the protein of interest. An amino acid consensus sequence is provided for the carrier protein domain, and syntheses of CoA-reporter analogs for tagging of heterologously expressed carrier protein domains are described. 4'-Phosphopantheteinyltransferase s can selectively transfer fluorescent CoA derivs. to carrier proteins (exemplified using VibB, a small protein from the Vibrio cholera vibriobactin biosynthesis machinery), and fluorescently labeled carrier protein domains are used to quantify post-translational modification in engineered systems.

IC ICM C12N
CC 7-1 (Enzymes)
Section cross-reference(s): 3, 9
ST biosynthetic enzyme analysis proteome labeled carrier protein; fatty acid synthase carrier protein analysis manipulation; polyketide

synthase carrier protein analysis manipulation; nonribosomal peptide synthase carrier protein analysis manipulation; CoA fluorescent deriv carrier protein proteome analysis

IT Proteins
RL: BUU (Biological use, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(ACP (acyl-carrier); anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT Proteins
RL: BUU (Biological use, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(ArCP (aryl carrier protein); anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT Proteins
RL: BUU (Biological use, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(PCP (peptidyl carrier protein); anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT Proteins
RL: BUU (Biological use, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(VibB; anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT Affinity chromatography
DNA sequence analysis
Gel electrophoresis
Mass spectrometry
Microarray technology
Protein sequence analysis
(anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT Enzymes, biological studies
RL: ANT (Analyte); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(biosynthetic; anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT Protein motifs
(carrier protein; anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT Proteins
RL: BUU (Biological use, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(carrier; anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT Infection
Virulence (microbial)
(determination of; anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT Natural products
RL: ANT (Analyte); ANST (Analytical study)
(determination of; anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT Post-translational processing
(quantification of; anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT 37278-30-1, Phosphopantetheinyltransferase
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(4'-, labeling of CoA-carrier protein domain-protein of

interest with; anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT 333956-92-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(Swern oxidation of; anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT 305372-39-8, Author's compound 1e from Table 1 (page 39) 491593-30-7, Author's compound 1f from Table 1 (page 39) 824393-56-8, Author's compound 1d from Table 1 (page 39)
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(affinity reporter; anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT 827065-87-2
RL: BUU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); USES (Uses)
(amino acid sequence of consensus carrier protein domain; anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT 9001-92-7, Proteinase
RL: ANT (Analyte); ANST (Analytical study)
(anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT 9045-77-6, Fatty acid synthase 79956-01-7, Polyketide synthase 115288-50-1, Nonribosomal peptide synthase
RL: ANT (Analyte); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT 85-61-0DP, Coenzyme A, fluorescent labeled derivs.
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT 56-17-7, Cystamine hydrochloride 91-20-3, Naphthalene, reactions 100-39-0, Benzyl bromide 599-04-2, D-Pantolactone
RL: RCT (Reactant); RACT (Reactant or reagent)
(anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT 1095-85-8P, 2-Tritylmercapto-ethylamine 20374-33-8P, (R)-3-Benzyloxy-4,4-dimethyl-dihydro-furan-2-one 253662-82-7P 277317-84-7P, (R)-3-Benzyloxy-4,4-dimethyl-tetrahydro-furan-2-ol 824393-45-5P 824393-46-6P, 3-(Fmoc-amino)-N-(2-tritylsulfanyl-ethyl)-propionamide 824393-47-7P, 2-(4-Methoxy-phenyl)-5,5-dimethyl-[1,3]dioxane-4-carboxylic acid[2-(2-tritylsulfanylethylcarbamoyl)ethyl]amide 824393-48-8P, (E,Z)-(S)-3-Benzyloxy-2,2-dimethyl-5-phenyl-pent-4-en-1-ol 824393-49-9P, (R)-2-Benzyloxy-4-(bis-benzyloxy-phosphoryloxy)-3,3-dimethyl-butyraldehyde 824393-50-2P, (R)-2-Benzyloxy-4-(bis-benzyloxy-phosphoryloxy)-3,3-dimethyl-butyric acid 824393-52-4P, Phosphoric acid dibenzyl ester (R)-3-benzyloxy-2,2-dimethyl-3-[2-(2-tritylsulfanyl-ethylcarbamoyl)-ethylcarbamoyl]-propyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT 496-65-1P, Pantetheine 2226-71-3P, Phosphopantetheine
RL: SPN (Synthetic preparation); PREP (Preparation)
(anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

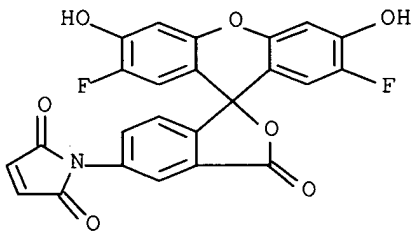
IT 76877-33-3, Author's compound 1c from Table 1 (page 39) 328085-55-8
, Author's compound 1b from Table 1 (page 39) 773859-49-7
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(fluorescent reporter; anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT 9031-09-8, Phosphotransferase 37288-21-4, Acyl carrier protein phosphodiesterase
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(labeling of CoA-carrier protein domain-protein of interest with; anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

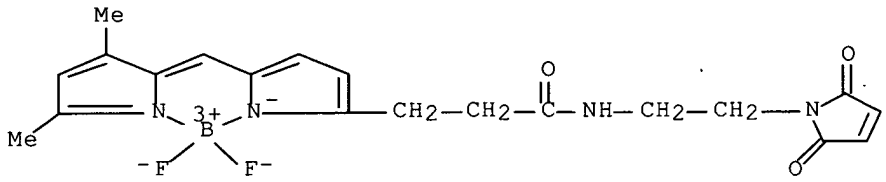
IT 826992-44-3 826992-45-4 826992-46-5 826992-47-6 826992-48-7
826992-49-8 826992-50-1 826992-51-2 826992-52-3 826992-53-4
826992-54-5 826992-55-6 826992-56-7 826992-57-8 826992-58-9
RL: PRP (Properties)
(unclaimed sequence; anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

IT 328085-55-8, Author's compound 1b from Table 1 (page 39)
773859-49-7
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(fluorescent reporter; anal. and manipulation of enzymes in biosynthetic proteomes using labeled carrier proteins)

RN 328085-55-8 CAPLUS
CN 1H-Pyrrole-2,5-dione, 1-(2',7'-difluoro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (CA INDEX NAME)



RN 773859-49-7 CAPLUS
CN Boron, [N-[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]-5-[(3,5-dimethyl-2H-pyrrol-2-ylidene-κN)methyl]-1H-pyrrole-2-propanamidato-κN1]difluoro-, (T-4)- (CA INDEX NAME)



L19 ANSWER 17 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:34516 CAPLUS Full-text
DOCUMENT NUMBER: 142:129786

TITLE: Assays for detection of phosphoinositide kinase and phosphatase activity
INVENTOR(S): Drees, Beth E.; Neilsen, Paul O.; Branch, Angie M.; Weipert, Amber; Hudson, Heather A.; Feng, Li; Prestwich, Glenn
PATENT ASSIGNEE(S): Echelon Biosciences Incorporated, USA
SOURCE: U.S. Pat. Appl. Publ., 39 pp., Cont.-in-part of U.S. Ser. No. 712,073.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

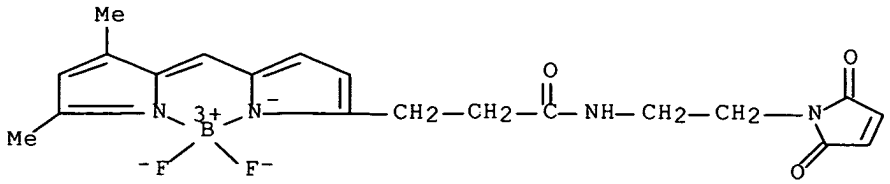
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005009124	A1	20050113	US 2004-850833	20040520
US 2003100028	A1	20030529	US 2001-991933	20011126
US 7067269	B2	20060627		
US 2004096923	A1	20040520	US 2003-712073	20031113

PRIORITY APPLN. INFO.:

US 2001-991933	A2	20011126
US 2002-426572P	P	20021115
US 2003-712073	A2	20031113

AB A method for detection of a lipid kinase or phosphatase is disclosed. The assay is preferably a competitive assay wherein the product lipid has a stronger affinity for a lipid detector protein than the substrate lipid. The lipid recognition motif is preferably a pleckstrin homol. (PH) domain. A representative assay comprises 4 steps. The first is enzyme-catalyzed cleavage of a substrate phosphoinositide. Water-soluble di-C8-phosphoinositides are used, which eliminates the need for liposomes formation and results in more consistent assay conditions. Secondly, the reaction is stopped by addition of a chelator. Then, a phosphoinositide- binding protein such as GST-Grp1 or GST-TAPP1 is added along with a fluorophore-labeled phosphoinositide tracer (e.g., FAM-PI(3,4,5)P3, TAMRA-I(1,3,4,5)P4, BODIPY-TMR-PI(3,4,5)P3). Finally, fluorescent polarization values are measured to determine the extent of the reaction.

IC ICM G01N033-53
INCL 435007920
CC 7-2 (Enzymes)
ST phosphoinositide kinase phosphatase detn Grp1 TAPP1 fluorophore labeled phosphatidylinositol
IT Fluorescent substances
(substrates labeled with; assays for detection of phosphoinositide kinase and phosphatase activity)
IT 773859-49-7, BODIPY FL N-(2-aminoethyl)maleimide
RL: RCT (Reactant); RACT (Reactant or reagent)
(BODIPY FL N-(2-aminoethyl)maleimide; assays for detection of phosphoinositide kinase and phosphatase activity)
IT 773859-49-7, BODIPY FL N-(2-aminoethyl)maleimide
RL: RCT (Reactant); RACT (Reactant or reagent)
(BODIPY FL N-(2-aminoethyl)maleimide; assays for detection of phosphoinositide kinase and phosphatase activity)
RN 773859-49-7 CAPLUS
CN Boron, [N-[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]-5-[(3,5-dimethyl-2H-pyrrol-2-ylidene-κN)methyl]-1H-pyrrole-2-propanamidato-κN1]difluoro-, (T-4)- (CA INDEX NAME)



L19 ANSWER 18 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:1069941 CAPLUS Full-text
DOCUMENT NUMBER: 142:193837
TITLE: Topology of the Outer Membrane Usher PapC Determined by Site-directed Fluorescence Labeling
AUTHOR(S): Henderson, Nadine S.; So, Stephane Shu Kin; Martin, Cheryl; Kulkarni, Ritwij; Thanassi, David G.
CORPORATE SOURCE: Department of Molecular Genetics and Microbiology, Center for Infectious Diseases, Stony Brook University, Stony Brook, NY, 11794-5120, USA
SOURCE: Journal of Biological Chemistry (2004), 279(51), 53747-53754
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In contrast to typical membrane proteins that span the lipid bilayer via transmembrane α-helixes, bacterial outer membrane proteins adopt a β-barrel architecture composed of antiparallel transmembrane β-strands. The topol. of outer membrane proteins is difficult to predict accurately using computer algorithms, and topol. mapping protocols commonly used for α-helical membrane proteins do not work for β-barrel proteins. The topol. of the PapC usher, an outer membrane protein required for assembly and secretion of P pili by the chaperone/usher pathway in uropathogenic Escherichia coli is presented here. An initial attempt to map PapC topol. by insertion of protease cleavage sites was largely unsuccessful due to lack of cleavage at most sites and the requirement to disrupt the outer membrane to identify periplasmic sites. Therefore a site-directed fluorescent labeling technique is adapted to permit topol. mapping of outer membrane proteins using small mol. probes in intact bacteria. Using this method, we demonstrated that PapC has the potential to encode up to 32 transmembrane β-strands. Based on exptl. evidence, it is proposed that the usher consists of an N-terminal β-barrel domain comprised of 26 β-strands and that a distinct C-terminal domain is not inserted into the membrane but is located instead within the lumen of the N-terminal β-barrel similar to the plug domains encoded by the outer membrane iron-siderophore uptake proteins.

CC 9-16 (Biochemical Methods)
Section cross-reference(s): 10
ST topol outer membrane usher PapC sitedirected fluorescence labeling mutation
IT Mutation
(insertion; topol. of outer membrane usher PapC determined by site-directed fluorescence labeling)
IT Proteins
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(membrane, PapC usher; topol. of outer membrane usher PapC determined by site-directed fluorescence labeling)

IT Organelle
(periplasm; topol. of outer membrane usher PapC determined by site-directed fluorescence labeling)

IT Fluorometry
(site-directed fluorescent labeling; topol. of outer membrane usher PapC determined by site-directed fluorescence labeling)

IT Escherichia coli
Eubacteria
Fluorescent indicators
Molecular topology
Mutation
β-Barrel
(topol. of outer membrane usher PapC determined by site-directed fluorescence labeling)

IT Probes (nucleic acid)
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(topol. of outer membrane usher PapC determined by site-directed fluorescence labeling)

IT Siderophores
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(topol. of outer membrane usher PapC determined by site-directed fluorescence labeling)

IT Protein degradation
(trypsin; topol. of outer membrane usher PapC determined by site-directed fluorescence labeling)

IT Conformation
(β-strand; topol. of outer membrane usher PapC determined by site-directed fluorescence labeling)

IT 9001-92-7, Proteinase
RL: NUU (Other use, unclassified); USES (Uses)
(TEV; topol. of outer membrane usher PapC determined by site-directed fluorescence labeling)

IT 52-90-4, Cysteine, analysis
RL: ANT (Analyte); ANST (Analytical study)
(topol. of outer membrane usher PapC determined by site-directed fluorescence labeling)

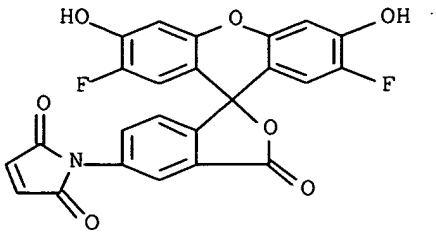
IT 328085-55-8, Oregon green 488 maleimide
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(topol. of outer membrane usher PapC determined by site-directed fluorescence labeling)

IT 118121-38-3
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(topol. of outer membrane usher PapC determined by site-directed fluorescence labeling)

IT 57-13-6, Urea, uses 1310-73-2, Sodium hydroxide, uses 7647-14-5, Sodium chloride, uses
RL: NUU (Other use, unclassified); USES (Uses)
(topol. of outer membrane usher PapC determined by site-directed fluorescence labeling)

IT 328085-55-8, Oregon green 488 maleimide
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(topol. of outer membrane usher PapC determined by site-directed fluorescence labeling)

RN 328085-55-8 CAPLUS
CN 1H-Pyrrole-2,5-dione, 1-(2',7'-difluoro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (CA INDEX NAME)

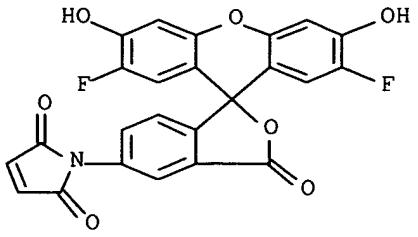


REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 19 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:1052415 CAPLUS Full-text
DOCUMENT NUMBER: 142:177101
TITLE: Design and Synthesis of a Bimodal Target-Specific Contrast Agent for Angiogenesis
AUTHOR(S): Dirksen, Anouk; Langereis, Sander; de Waal, Bas F. M.; van Genderen, Marcel H. P.; Meijer, E. W.; de Lussanet, Quido G.; Hackeng, Tilman M.
CORPORATE SOURCE: Laboratory of Macromolecular and Organic Chemistry, Eindhoven University of Technology, Eindhoven, 5600 MB, Neth.
SOURCE: Organic Letters (2004), 6(26), 4857-4860
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:177101

AB A bimodal target-specific contrast agent based on a cyclic peptide containing the target-specific NGR sequence, gadolinium(III), diethylenetriaminepentaacetic acid, and Oregon Green 488, suitable for both MR imaging and optical imaging of angiogenesis is developed. The synthetic strategy for this target-specific contrast agent exploits the use of highly efficient, chemoselective reactions, such as native chemical ligation, and gives a straightforward approach for double labeling of peptides in general.

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 9
IT 108-98-5, Thiophenol, reactions 10138-52-0, Gadolinium(III) chloride 288144-38-7 328085-55-8 832099-89-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of a bimodal target-specific contrast agent for angiogenesis)
IT 328085-55-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of a bimodal target-specific contrast agent for angiogenesis)
RN 328085-55-8 CAPLUS
CN 1H-Pyrrole-2,5-dione, 1-(2',7'-difluoro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 20 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:173706 CAPLUS Full-text
DOCUMENT NUMBER: 141:327625
TITLE: Manipulation of Carrier Proteins in Antibiotic Biosynthesis
AUTHOR(S): La Clair, James J.; Foley, Timothy L.; Schegg, Tracy R.; Regan, Conor M.; Burkart, Michael D.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of California, La Jolla, CA, 92093, USA
SOURCE: Chemistry & Biology (2004), 11(2), 195-201
CODEN: CBOLE2; ISSN: 1074-5521
PUBLISHER: Cell Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Engineering biosynthetic pathways into suitable host organisms has become an attractive venue for the design, evaluation, and production of small mol. therapeutics. Polyketide (PK) and nonribosomal peptide (NRP) synthases have been of particular interest due to their modular structure, yet routine cloning and expression of these enzymes remains challenging. Here we describe a method to covalently label carrier proteins from PK and NRP synthases using the enzymic transfer of a modified CoA analog by a 4'-phosphopantetheinyltransferase. Using this method, carrier proteins can be loaded with single fluorescent or affinity reporters, providing novel entry for protein visualization, Western blot identification, and affinity purification Application of these methods provides an ideal tool to track and quantify metabolically engineered pathways. Such techniques are valuable to measure protein expression, solubility, activity, and native posttranslational modification events in heterologous systems.

CC 7-8 (Enzymes)
Section cross-reference(s): 9

IT Enzyme functional sites
(carrier protein domain; labeling carrier protein domains within polyketide and nonribosomal peptide synthases with fluorescent or affinity reporter CoA mols. for identification and isolation of the synthases)

IT Affinity chromatography
Immunoblotting
Post-translational processing
(labeling carrier protein domains within polyketide and nonribosomal peptide synthases with fluorescent or affinity reporter CoA mols. for identification and isolation of the synthases)

IT 79956-01-7DP, Polyketide synthase, complexes with maleimide reporter CoA derivs. 115288-50-1DP, Nonribosomal peptide synthase, complexes with maleimide reporter CoA derivs. 756898-07-4DP, complexes with carrier

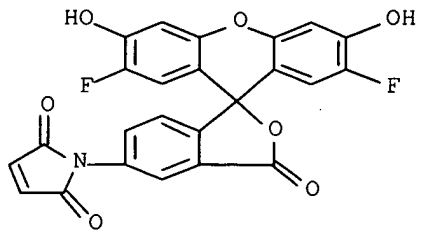
domain of polyketide or nonribosomal peptide synthases 771586-68-6DP, complexes with carrier domain of polyketide or nonribosomal peptide synthases 771586-69-7DP, complexes with carrier domain of polyketide or nonribosomal peptide synthases 771586-70-0DP, complexes with carrier domain of polyketide or nonribosomal peptide synthases 771586-71-1DP, complexes with carrier domain of polyketide or nonribosomal peptide synthases 773859-50-0DP, complexes with carrier domain of polyketide or nonribosomal peptide synthases
RL: ANT (Analyte); PUR (Purification or recovery); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)
(labeling carrier protein domains within polyketide and nonribosomal peptide synthases with fluorescent or affinity reporter CoA mols. for identification and isolation of the synthases)

IT 37278-30-1
RL: BSU (Biological study, unclassified); CAT (Catalyst use); BIOL (Biological study); USES (Uses)
(labeling carrier protein domains within polyketide and nonribosomal peptide synthases with fluorescent or affinity reporter CoA mols. for identification and isolation of the synthases)

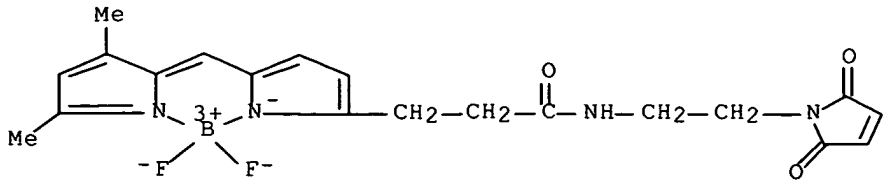
IT 85-61-0, Coenzyme A, reactions 55145-14-7, N-(7-Dimethylamino-4-methylcoumarin-3-yl)maleimide 116919-18-7 305372-39-8 328085-55-8, Oregon green 488 maleimide 491593-30-7 773859-49-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(labeling carrier protein domains within polyketide and nonribosomal peptide synthases with fluorescent or affinity reporter CoA mols. for identification and isolation of the synthases)

IT 328085-55-8, Oregon green 488 maleimide 773859-49-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(labeling carrier protein domains within polyketide and nonribosomal peptide synthases with fluorescent or affinity reporter CoA mols. for identification and isolation of the synthases)

RN 328085-55-8 CAPLUS
CN 1H-Pyrrole-2,5-dione, 1-(2',7'-difluoro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (CA INDEX NAME)



RN 773859-49-7 CAPLUS
CN Boron, [N-[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethyl]-5-[(3,5-dimethyl-2H-pyrrol-2-ylidene-κN)methyl]-1H-pyrrole-2-propanamidato-κN1]difluoro-, (T-4)- (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:662572 CAPLUS Full-text
DOCUMENT NUMBER: 139:288140
TITLE: Activation of Human Acid Sphingomyelinase through Modification or Deletion of C-terminal Cysteine
AUTHOR(S): Qiu, Huawei; Edmunds, Tim; Baker-Malcolm, Jennifer; Karey, Kenneth P.; Estes, Scott; Schwarz, Cordula; Hughes, Heather; Van Patten, Scott M.
CORPORATE SOURCE: Cell and Protein Therapeutics R & D Department, Genzyme Corp., Framingham, MA, 01701, USA
SOURCE: Journal of Biological Chemistry (2003), 278(35), 32744-32752
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

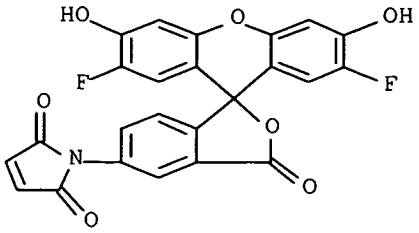
AB One form of Niemann-Pick disease is caused by a deficiency in the enzymic activity of acid sphingomyelinase. During efforts to develop an enzyme replacement therapy based on a recombinant form of human acid sphingomyelinase (rhASM), purified prepns. of the recombinant enzyme were found to have substantially increased specific activity if cell harvest media were stored for several weeks at -20 °C prior to purification This increase in activity was found to correlate with the loss of the single free thiol on rhASM, suggesting the involvement of a cysteine residue. It was demonstrated that a variety of chemical modifications of the free cysteine on rhASM all result in substantial activation of the enzyme, and the modified cysteine responsible for this activation was shown to be the C-terminal residue (Cys629). Activation was also achieved by copper-promoted dimerization of rhASM (via cysteine) and by C-terminal truncation using carboxypeptidase Y. The role of the C-terminal cysteine in activation was confirmed by creating mutant forms of rhASM in which this residue was either deleted or replaced by a serine, with both forms having substantially higher specific activity than wild-type rhASM. These results indicate that purified rhASM can be activated in vitro by loss of the free thiol on the C-terminal cysteine via chemical modification, dimerization, or deletion of this amino acid residue. This method of activation is similar to the cysteine switch mechanism described previously for matrix metalloproteinases and could represent a means of posttranslational regulation of ASM activity in vivo.

CC 7-5 (Enzymes)
IT 328085-55-8, Oregon Green 488 maleimide
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(chemical modification of C-terminal Cys629 with Oregon Green 488 maleimide promotes activation of human acid sphingomyelinase)
IT 328085-55-8, Oregon Green 488 maleimide

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(chemical modification of C-terminal Cys629 with Oregon Green 488 maleimide promotes activation of human acid sphingomyelinase)

RN 328085-55-8 CAPLUS

CN 1H-Pyrrole-2,5-dione, 1-(2',7'-difluoro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (CA INDEX NAME)



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

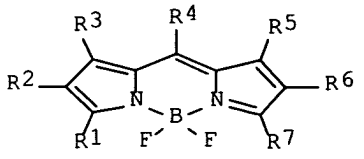
L19 ANSWER 22 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:42536 CAPLUS Full-text
DOCUMENT NUMBER: 138:103273
TITLE: Two-photon absorbing dipyrromethene boron difluoride dyes and their applications
INVENTOR(S): Meltola, Niko; Soini, Aleksi
PATENT ASSIGNEE(S): Arctic Diagnostics Oy, Finland
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003005030	A1	20030116	WO 2002-FI586	20020701
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002319326	A1	20030121	AU 2002-319326	20020701
EP 1402263	A1	20040331	EP 2002-748895	20020701
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
CN 1526071	A	20040901	CN 2002-813441	20020701
JP 2004533626	T	20041104	JP 2003-510955	20020701
RU 2296333	C2	20070327	RU 2004-102687	20020701
US 2004157231	A1	20040812	US 2003-482205	20031229

PRIORITY APPLN. INFO.: FI 2001-1439 A 20010702
US 2001-301788P P 20010702
WO 2002-FI586 W 20020701

OTHER SOURCE(S): MARPAT 138:103273

GI



I

AB The invention relates to a separation free bioanal. assay method for measuring an analyte from a biol. fluid or suspension comprising of microparticles as a bioaffinity binding solid phase, a biospecific secondary reagent labeled with a two-photon fluorescent dipyrromethene boron difluoride dye, focusing the laser into the reaction suspension measuring two-photon excited fluorescence from single microparticles when they randomly float or are guided by the radiation pressure of the excitation laser through the focal volume of the laser beam using a two-photon fluorescent dipyrromethene boron difluoride dye. Dye has the structure II. At least one of the groups R1, R2, R3, R4, R5, R6 or R7 is substituted to yield a chemical reactive group that can be used for selective covalent linkage to other mols. and at least one of the groups R1, R2, R3, R4, R5, R6, R7 is substituted to yield a water-solubilizing group.

IC ICM G01N033-543
ICS C09B062-44

CC 9-5 (Biochemical Methods)
Section cross-reference(s): 41

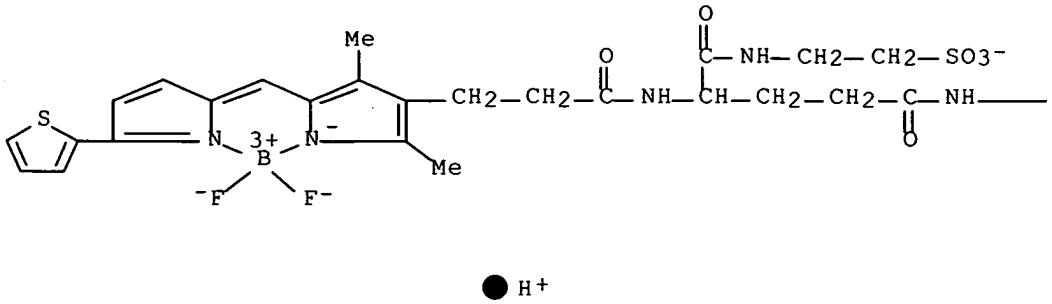
IT 66145-58-2P 87047-24-3P 485393-51-9P 485393-52-0P 485393-53-1P
485393-54-2P 485393-55-3P 485393-56-4P 485393-57-5P 485393-58-6P
485393-59-7P 485393-60-0P 485393-61-1P 485393-62-2P 485393-63-3P
485393-64-4P 485393-65-5P 485393-66-6P
RL: ARU (Analytical role, unclassified); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent)
(two-photon absorbing dipyrromethene boron difluoride dyes and their applications)

IT 485393-66-6P
RL: ARU (Analytical role, unclassified); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent)
(two-photon absorbing dipyrromethene boron difluoride dyes and their applications)

RN 485393-66-6 CAPLUS

CN Borate(1-), [2-[[(2S)-5-[[2-[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino]ethyl]amino]-2-[[3-[2,4-dimethyl-5-[[5-(2-thienyl)-2H-pyrrol-2-ylidene-κN]methyl]-1H-pyrrol-3-yl-κN]-1-oxopropyl]amino]-1,5-dioxopentyl]amino]ethanesulfonato(2-)]difluoro-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A



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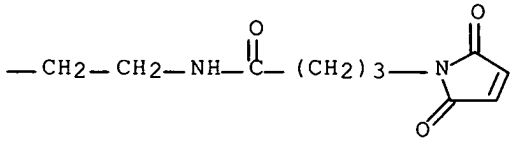


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 23 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:42337 CAPLUS Full-text
DOCUMENT NUMBER: 138:91395
TITLE: Method for increasing hydrophilicity of fluorescent label compounds, and their use
INVENTOR(S): Meltola, Niko; Soini, Aleksi
PATENT ASSIGNEE(S): Arctic Diagnostics Oy, Finland
SOURCE: PCT Int. Appl., 46 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003004569	A1	20030116	WO 2002-FI581	20020701
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002321334	A1	20030121	AU 2002-321334	20020701
EP 1401962	A1	20040331	EP 2002-755031	20020701

EP 1401962	B1	20060913			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK					
JP 2004533533	T	20041104	JP 2003-510732		20020701
AT 339475	T	20061015	AT 2002-755031		20020701
US 2004147728	A1	20040729	US 2003-482057		20031229
US 7198958	B2	20070403			
PRIORITY APPLN. INFO.:			FI 2001-1438	A	20010702
			US 2001-301831P	P	20010702
			WO 2002-FI581	W	20020701

OTHER SOURCE(S): MARPAT 138:91395

AB The invention relates to fluorescent label compds. in the form of dipyrrometheneboron difluoride dye derivs. containing NHCH(CH2CH2Z)CONHY or NHCZCH2CH2CONHY groups, wherein Z is a reactive group and Y is a water-solubilizing moiety or CH2CH2SO3X, with X being a cation. The invention also relates to the use of the compds. in bioanal. assays and cytol. or histol. staining methods. The invention further relates to a method for increasing the hydrophilicity of fluorescent compds. In an example, a glutamic acid-taurine linker, HO2CCH2CH2CH(NH2)CONHCH2CH2SO3H, was prepared and condensed with 4,4-difluoro-5-(2-thienyl)-1,3-dimethyl-4- bora-3a,4a-diaza-s-indacene-2-propionic acid succinimidyl ester and the product was then re-esterified with N-hydroxysuccinimide to give a fluorescent compound suitable for labeling of mouse IgG anti-AFP.

IC ICM C09B062-44

CC 41-5 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)
Section cross-reference(s): 9, 78

ST dipyrrometheneboron difluoride fluorescent biomol labeling dye prodn hydrophilic

IT Fluorescent dyes
Fluorescent indicators
(production of hydrophilic dipyrrometheneboron difluoride fluorescent biomol. labeling dyes)

IT 485393-58-6P 485397-10-2P
RL: BUU (Biological use, unclassified); IMF (Industrial manufacture); BIOL (Biological study); PREP (Preparation); USES (Uses)
(dye; production of hydrophilic dipyrrometheneboron difluoride fluorescent biomol. labeling dyes)

IT 485393-57-5P
RL: BUU (Biological use, unclassified); IMF (Industrial manufacture); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(dye; production of hydrophilic dipyrrometheneboron difluoride fluorescent biomol. labeling dyes)

IT 87047-24-3P 485393-56-4P 485393-63-3P 485393-64-4P 485397-09-9P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; production of hydrophilic dipyrrometheneboron difluoride fluorescent biomol. labeling dyes)

IT 485393-59-7P 485393-60-0P 485393-61-1P 485393-62-2P 485393-65-5P 485393-66-6P
RL: IMF (Industrial manufacture); PREP (Preparation)
(production of hydrophilic dipyrrometheneboron difluoride fluorescent biomol. labeling dyes)

IT 107-15-3, Ethylenediamine, reactions 107-35-7, Taurine 463-71-8, Thiophosgene 6066-82-6, N-Hydroxysuccinimide 13472-00-9, 4-(2-Aminoethyl)aniline 32886-55-8 209112-21-0 485393-55-3 485396-99-4 485397-11-3 485397-12-4 485397-13-5 485397-14-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; production of hydrophilic dipyrrometheneboron

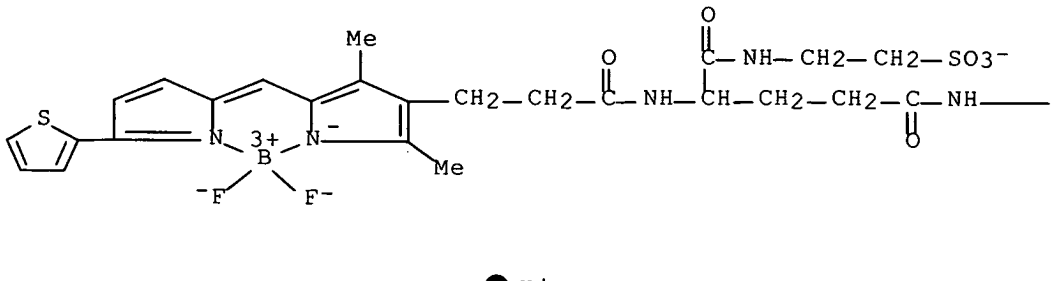
difluoride fluorescent biomol. labeling dyes)

IT 485393-66-6P
RL: IMF (Industrial manufacture); PREP (Preparation)
(production of hydrophilic dipyrromethene boron difluoride fluorescent biomol. labeling dyes)

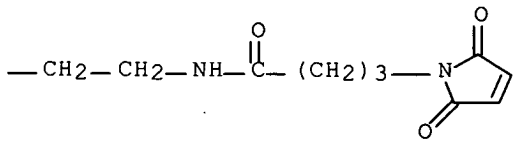
RN 485393-66-6 CAPLUS

CN Borate(1-), [2-[[(2S)-5-[[2-[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino]ethyl]amino]-2-[[3-[2,4-dimethyl-5-[[5-(2-thienyl)-2H-pyrrol-2-ylidene-κN]methyl]-1H-pyrrol-3-yl-κN]-1-oxopropyl]amino]-1,5-dioxopentyl]amino]ethanesulfonato(2-)]difluoro-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 24 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:163416 CAPLUS Full-text
DOCUMENT NUMBER: 134:202253
TITLE: Photoluminescent sensors of chemical analytes
INVENTOR(S): Thompson, Richard B.; Feliccia, Vincent L.; Maliwal, Badri P.; Fierke, Carol A.
PATENT ASSIGNEE(S): University of Maryland, Baltimore, USA
SOURCE: U.S., 61 pp., Cont.-in-part of U.S. Ser. No. 71,351.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 6197258	B1	20010306	US 1999-273303	19990319
US 5952236	A	19990914	US 1996-736904	19961025
US 6284544	B1	20010904	US 1998-71351	19980430

PRIORITY APPLN. INFO.:

US 1996-736904	A2	19961025
US 1997-45289P	P	19970501
US 1998-78597P	P	19980319
US 1998-71351	A2	19980430
US 1998-83868P	P	19980501
US 1995-5879P	P	19951026

AB The invention described in detail herein relates to the detection, determination, and quantitation of certain ions and small mols. in solution The invention specifically relates to improvements in the area of photoluminescent sensors for use in a detection scheme involving the alteration of a photoluminescent label or moiety attached to or associated with an analyte binding macromol. One may use the changes in photoluminescence lifetime, changes in ratios of photoluminescence intensity or changes in photoluminescence polarization (anisotropy) to determine the analyte. The photoluminescence change measured correlates to the concentration of the ion or mol. in solution

IC ICM G01N033-20
ICS C12Q001-00

INCL 422082070

CC 79-2 (Inorganic Analytical Chemistry)
Section cross-reference(s): 9, 61

ST photoluminescent sensor analyte; metal detn water luminescence labeled biomol

IT Fluorescence quenching
Fluorescent substances
Luminescence spectroscopy
Optical sensors
Polarized luminescence
(metal ion determination in aqueous samples by photoluminescent sensors based on fluorescently labeled macromols. with metal ion binding site)

IT Metals, analysis
RL: ANT (Analyte); ANST (Analytical study)
(metal ion determination in aqueous samples by photoluminescent sensors based on fluorescently labeled macromols. with metal ion binding site)

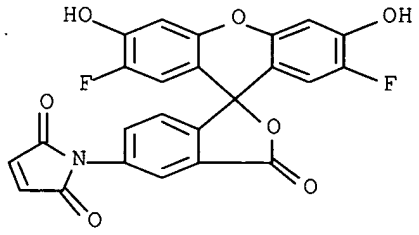
IT Macromolecular compounds
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(metal ion determination in aqueous samples by photoluminescent sensors based on fluorescently labeled macromols. with metal ion binding site)

IT 138219-58-6, Dapoxyl sulfonamide
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(Dapoxyl sulfonamide; metal ion determination in aqueous samples by photoluminescent sensors based on fluorescently labeled macromols. with metal ion binding site)

IT 328085-55-8, Oregon Green 488 maleimide
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(Oregon Green 488 maleimide; metal ion determination in aqueous samples by photoluminescent sensors based on fluorescently labeled macromols. with metal ion binding site)

IT 155862-97-8, PyMPO-maleimide
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(PyMPO-maleimide; metal ion determination in aqueous samples by photoluminescent sensors based on fluorescently labeled macromols. with metal ion binding site)

IT 7732-18-5, Water, analysis
RL: AMX (Analytical matrix); ANST (Analytical study)
(metal ion determination in aqueous samples by photoluminescent sensors based on
fluorescently labeled macromols. with metal ion binding site)
IT 7440-02-0, Nickel, analysis 7440-43-9, Cadmium, analysis 7440-48-4, Cobalt, analysis 7440-50-8, Copper, analysis 7440-66-6, Zinc, analysis
RL: ANT (Analyte); ANST (Analytical study)
(metal ion determination in aqueous samples by photoluminescent sensors based on
fluorescently labeled macromols. with metal ion binding site)
IT 9001-03-0, Carbonic anhydrase 91366-67-5 244207-05-4 244779-68-8 327623-77-8
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(metal ion determination in aqueous samples by photoluminescent sensors based on
fluorescently labeled macromols. with metal ion binding site)
IT 328085-55-8, Oregon Green 488 maleimide
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(Oregon Green 488 maleimide; metal ion determination in aqueous samples by photoluminescent sensors based on fluorescently labeled macromols. with metal ion binding site)
RN 328085-55-8 CAPLUS
CN 1H-Pyrrole-2,5-dione, 1-(2',7'-difluoro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl)- (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 25 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:198648 CAPLUS Full-text
DOCUMENT NUMBER: 124:337016
TITLE: Wave chemistry: 2-(4'-azido-3',5',6'-trifluoro-2'-pyridyl)-aminoethylamine as a key photoactivatable building block with wide biological applications
AUTHOR(S): Nungaray, Jesus; Meziane-Cherif, Djalal; LeGoffic, Francois
CORPORATE SOURCE: Lab. Biorganique Biotechnologies, Ecole Nationale Superieure Chim. Paris, Paris, 75231, Fr.
SOURCE: Synthetic Communications (1996), 26(7), 1273-87
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Dekker
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:337016

AB The synthesis of the title compound is described as well as a series of derivs. with wide biol. applications.

CC 9-5 (Biochemical Methods)
Section cross-reference(s): 27

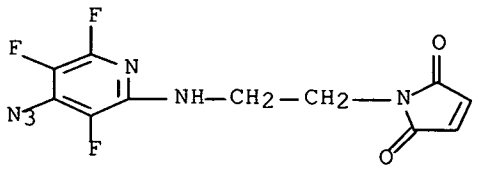
IT Membrane, biological
Photoaffinity labeling
((azidotrifluoropyridyl)aminoethylamine as photoactivatable compound for biol. applications)

IT 176724-46-2P 176724-47-3P 176724-50-8P 176724-51-9P
176724-52-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
((azidotrifluoropyridyl)aminoethylamine as photoactivatable compound for biol. applications)

IT 176724-46-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
((azidotrifluoropyridyl)aminoethylamine as photoactivatable compound for biol. applications)

RN 176724-46-2 CAPLUS

CN 1H-Pyrrole-2,5-dione, 1-[2-[(4-azido-3,5,6-trifluoro-2-pyridinyl)amino]ethyl]- (CA INDEX NAME)



L19 ANSWER 26 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1993:582860 CAPLUS Full-text
DOCUMENT NUMBER: 119:182860
TITLE: Chemically reactive dipyrromethene boron difluoride dyes and their conjugates
INVENTOR(S): Kang, Hee Chol; Haugland, Richard P.
PATENT ASSIGNEE(S): Molecular Probes, Inc., USA
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 11
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9309185	A1	19930513	WO 1992-US8350	19920930
W: CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE				
US 5274113	A	19931228	US 1991-786767	19911101
EP 612336	A1	19940831	EP 1992-922004	19920930
EP 612336	B1	19980107		
R: AT, BE, CH, DE, FR, GB, LI, NL				
AT 161871	T	19980115	AT 1992-922004	19920930
CA 2122627	C	20020611	CA 1992-2122627	19920930
PRIORITY APPLN. INFO.:			US 1991-786767 A	19911101

WO 1992-US8350 W 19920930

OTHER SOURCE(S): MARPAT 119:182860

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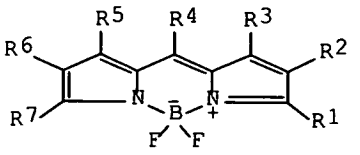


I

AB Fluorescent dyes I [R1-R7 = H, halogen, (un)substituted C1-5 alkyl, (un)substituted aryl, SO3H, bathochromic group, LmG; ≥1 of R1-R7 = LmG; G = reactive group; L = (un)substituted C1-5 alkylene or arylene, bathochromic linking group; m = 0, 1; ≥1 bathochromic group is present] having emission maximum .gtorsim.550 nm in MeOH and quantum yield .gtorsim.0.1, form conjugates with nucleic acids, proteins, carbohydrates, etc. Thus, POCl3 was added to a solution of 2-formyl-5-(2-thienyl)pyrrole and 2-(2-methoxycarbonylethyl)pyrrole in CH2Cl2 and the solution stirred 16 h at room temperature, neutralized with iso-Pr2NEt, and treated with BF3.OEt2 to give 52% I (R1 = CH2CH2CO2Me, R2-R6 = H, R7 = 2-thienyl), which was hydrolyzed with H3PO4 and reesterified with N-hydroxysuccinimide. The succinimidyl ester formed a conjugate with 5-(3-aminoallyl)-2'- deoxyuridine-5'-triphosphate ammonium salt which showed an absorption maximum at 558.6 nm and an emission maximum at 570 nm in pH 7 phosphate buffer.

IC ICM C09B057-00
ICS C07F005-02; A61K031-40; A61K031-69

CC 41-5 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)
Section cross-reference(s): 9

ST dipyrromethene boron fluoride dye conjugate; nucleotide fluorescent dye conjugate; labeling fluorescent dye

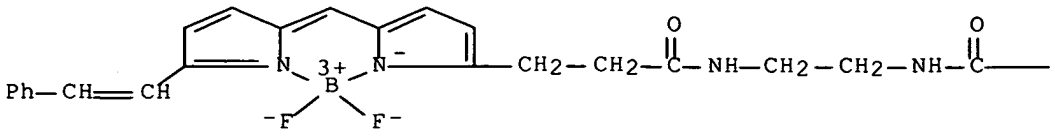
IT 148250-82-2P 150152-61-7P 150152-62-8P 150152-63-9P 150152-64-0P
150152-65-1P 150152-66-2P 150152-67-3P 150152-68-4P 150152-69-5P
150152-70-8P 150152-71-9P 150152-72-0P 150173-71-0P 150173-72-1P
150173-73-2P 150173-74-3P 150173-75-4P 150173-76-5P 150173-77-6P
150173-78-7P 150173-79-8P 150173-80-1P 150173-81-2P 150173-82-3P
150173-83-4P 150173-84-5P 150173-85-6P 150173-86-7P 150173-87-8P
150173-88-9P 150173-89-0P 150173-90-3P 150173-91-4P 150173-92-5P
150173-93-6P 150173-94-7P 150173-95-8P 150173-96-9P
150173-97-0P 150173-98-1P 150173-99-2P 150174-00-8P 150174-01-9P
150174-02-0P 150174-03-1P 150237-60-8P
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of, as fluorescent dye for labeling biomols.)

IT 150173-93-6P
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of, as fluorescent dye for labeling biomols.)

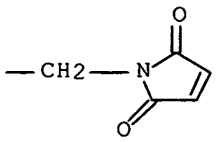
RN 150173-93-6 CAPLUS

CN Boron, [N-[2-[[(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)acetyl]amino]ethyl]-5-[[5-[(1E)-2-phenylethenyl]-2H-pyrrol-2-ylidene-κN]methyl]-1H-pyrrole-2-propanamidato-κN1]difluoro-, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L19 ANSWER 27 OF 27 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1993:581068 CAPLUS Full-text
DOCUMENT NUMBER: 119:181068
TITLE: A synthesis of 7α-substituted estradiols: synthesis and biological evaluation of a 7α-pentyl-substituted BODIPY fluorescent conjugate and a fluorine-18-labeled 7α-pentylestradiol analog
AUTHOR(S): French, Andrew N.; Wilson, Scott R.; Welch, Michael J.; Katzenellenbogen, John A.
CORPORATE SOURCE: Dep. Chem., Univ. Illinois, Urbana, IL, 61801, USA
SOURCE: Steroids (1993), 58(4), 157-69
CODEN: STEDAM; ISSN: 0039-128X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:181068
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB In an effort to assist in the preparation of ligands for the study of the estrogen receptor (ER), a new synthesis of 7α-substituted estradiols, e.g. I and II, was developed. The key step in the synthesis involves a copper-catalyzed, α-selective, 1,6-conjugate addition of 4-pentenylmagnesium bromide to dehydrotestosterone derivative III to give 6α-pentenyl derivative IV along with a small amount of the 6β-diastereoisomer. IV was oxidized with DDQ to give the corresponding 1,2-dehydro derivative, which underwent reductive aromatization to give 7α-pentenylestradiol V. The α-stereoselectivity of addition reaction in the testosterone series, compared with the 19-nortestosterone series, is significantly improved by the presence of the C-19 Me group, which shields the beta face from attack. A key intermediate was functionalized further by substitution with fluorine-18 to provide a potential imaging agent for positron emission tomog., and by conjugation with a BODIPY

fluorophore to make a fluorescent probe for the estrogen receptor. The synthesis and biol. evaluation of these analogs is presented, as well as a discussion of the improvements in the synthetic procedure.

CC 32-3 (Steroids)
Section cross-reference(s): 2, 75

ST estradiol substituted deriv; pentylestradiol fluorine 18 labeled BODIPY conjugate; BODIPY fluorescent conjugate pentylestradiol; estrogen receptor substituted estradiol deriv

IT Receptors
RL: PRP (Properties)
(estrogen, binding affinity of, with pentylestradiol BODIPY fluorescent conjugate and fluorine-18-labeled pentylestradiol analog)

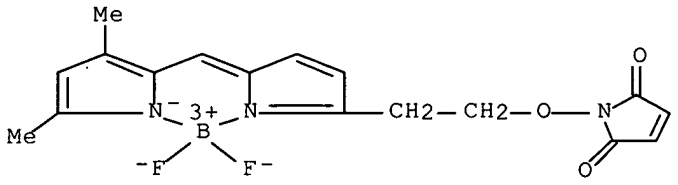
IT Estrogens
RL: PRP (Properties)
(receptors, binding affinity of, with pentylestradiol BODIPY fluorescent conjugate and fluorine-18-labeled pentylestradiol analog)

IT 150413-50-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of, with (aminopentyl)estradiol)

IT 150413-50-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of, with (aminopentyl)estradiol)

RN 150413-50-6 CAPLUS

CN Boron,· [1-[2-[2-[(3,5-dimethyl-1H-pyrrol-2-yl)methylene]-2H-pyrrol-5-yl]ethoxy]-1H-pyrrole-2,5-dionato]difluoro-, (T-4)- (9CI) (CA INDEX NAME)



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L4              STR
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